*Electronic Supplementary Information*

# Copper-mediated C($sp^3$)-H azidation with $Me_3SiN_3$: synthesis of imidazoles from ketones and aldehydes

Zeqiang Xie, ‡ [a] Jiaojiao Deng, ‡ [b], Zhiping Qiu,[b] Juan Li*[b] and Qiang Zhu*[a]

[a]*State Key Laboratory of Respiratory Disease, Guangzhou Institutes of Biomedicine and Health, Chinese Academy of Sciences, 190 Kaiyuan Avenue, Guangzhou 510530, China.*
[b]*Department of Chemistry, Jinan University, Huangpu Road West 601, Guangzhou 510632, China.*
Email: *zhu_qiang@gibh.ac.cn; tchjli@jnu.edu.cn*

## Table of Contents

# I. General Information

All reagents were purchased without further purification unless otherwise noted. Reactions were monitored using thin-layer chromatography (TLC) on commercial silica gel plates (GF254). Visualization of the developed plates was performed under UV light (254 nm). Flash column chromatography was performed on silica gel (200-300 mesh). $^{1}H$ and $^{13}C$ NMR spectra were recorded on a 400 or 500 MHz spectrometer. Chemical shifts (δ) were reported in ppm referenced to an internal tetramethylsilane standard or the DMSO-$d_6$ residual peak (δ 2.50) for $^{1}H$ NMR. Chemical shifts of $^{13}C$ NMR were reported relative to DMSO-$d_6$ (δ 39.5). The following abbreviations were used to describe peak splitting patterns when appropriate: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Coupling constants, *J*, were reported in Hertz unit (Hz). High resolution mass spectra (HRMS) were obtained on an ESI-LC-MS/MS spectrometer.

# II. General Procedures and Optimization of the Reaction Conditions

Substrates **1** were prepared according to literature reported procedures.[1]

## (a) General Procedure for the Synthesis of 3

To a Schlenk tube were added ketone **1** (0.4 mmol)**,** $Cu(TFA)_2xH_2O$ (0.24 mmol), PivOH (0.2 mmol) and DCB (1.3 mL). Then, the tube was vacuumed and refilled with argon for 3 times. A solution of aldehyde **2** (0.2 mmol) in 0.2 mL of DCB was added via a syringe. The reaction mixture was stirred at 110 $^{o}$C, followed by addition of a solution of $TMSN_3$ (0.6 mmol, 3.0 equiv) in 0.5 mL of DCB via a syringe pump during 1.25 h. The reaction was stirred for another 4.75 h at this temperature. After cooling down, saturated aqueous NaCl (10 mL), $NH_4$·OH (1 mL) and EtOAc (10 mL) were added to the reaction mixture. The aqueous phase was further extracted with EtOAc (2 × 10 mL). The combined organic layers were dried over anhydrous $Na_2SO_4$ and concentrated. The residue was purified by flash chromatography to provide the desired product **3**.

# III. DFT Calculation

## (a) Computational Details

The molecular geometries of the complexes were optimized, using DFT, at the M06 level. [2] Frequency calculations at the same level of theory were also performed to identify all the stationary points as minima (zero imaginary frequencies) or transition states (one imaginary frequency) as well as to provide the free energies at 298.15 K. The IRC[3] analysis was performed to confirm that all stationary points were smoothly connected to each other. Cu atoms were described using the LANL2DZ basis set, including a double-valence basis set with the Hay and Wadt effective core potential.[4] Polarization functions were added for Cu ($\zeta_f$ = 3.525)[5] atom. The 6-31G*[6] basis set was used for the other atoms. In the polarizable continuum model (PCM) calculations, the SDD basis set was used for the Cu atom and the 6-311++G** basis set for the other atoms. All calculations were performed using Gaussian 09 packages.[7]

One may question whether the electronic and steric effects on the reaction mechanism of $Cu(TFA)_2$ is well modeled. We did a testing calculation using $Cu(TFA)_2$ for the **H** and the rate-determining transition states **TS3**. We found that the free energy of **TS3** for the $Cu(OAc)_2$ and $Cu(TFA)_2$ models are almost the same (29.6 versus 29.2 kcal/mol) relative to **H**. The results show that the electronic and steric effects of $Cu(TFA)_2$ does not affect the relative energies significantly, suggesting that the results derived from the $Cu(OAc)_2$ models are qualitatively valid.

To confirm that C($sp^3$)−H azidation product was a plausible reaction intermediate, density functional theory (DFT) calculations were conducted using $Cu(OAc)_2$ in place of $Cu(TFA)_2$ as a model catalyst to reduce the computational cost (see details in the ESI). Protonation of 1,2-diphenylethanone, calculated to be exergonic by 145 kcal/mol, formed the cation intermediate **A**. As shown in Figure 1, **A** was taken as the reference point. $Me_3SiN_3$ attacks the carbonium ion of **A** to complete the first C−N linkage via the transition state **TS1**,[8] followed by release of $Me_3SiOH$ to give **C** via the transition state **TS2**. Next, Cu coordinates to the terminal N atom of the azido group, then $N_2$ is liberated through the transition state **TS3**. Subsequently, the intermediate **E** is tautomerized to **G** via two transition states **TS4** and **TS5**. The coordination of $Me_3SiN_3$ to Cu then leads to the formation of intermediate **H**, which then release $Me_3SiOH$ to give **I** via **TS6**. The second C−N bond-formation through reductive elimination of the Cu(III) intermediate **I** via **TS7** occurs, followed by $N_2$ loss via **TS8**.[9] In the following step, benzaldehyde approaches the Cu

centre via **TS9** with the third C−N bond connected. The following dehydration and C−H-bond-breaking steps take place via the transition state **TS10** and **TS11**, respectively. Finally, the fourth C−N bond-forming step via **TS12** occurs delivering the final product **3b**. Our calculations indicate that the $N_2$ liberation step via **TS3** is rate-determining and the overall energy barrier is 29.6 kcal/mol. The direct amination of the methylene group is also calculated. However, the overall free energy barrier (33.9 kcal/mol) for direct amination pathway is determined to be 4.3 kcal/mol higher than that of pathway shown in Figure S1.

## (b) The Calculated Free Energy Profiles

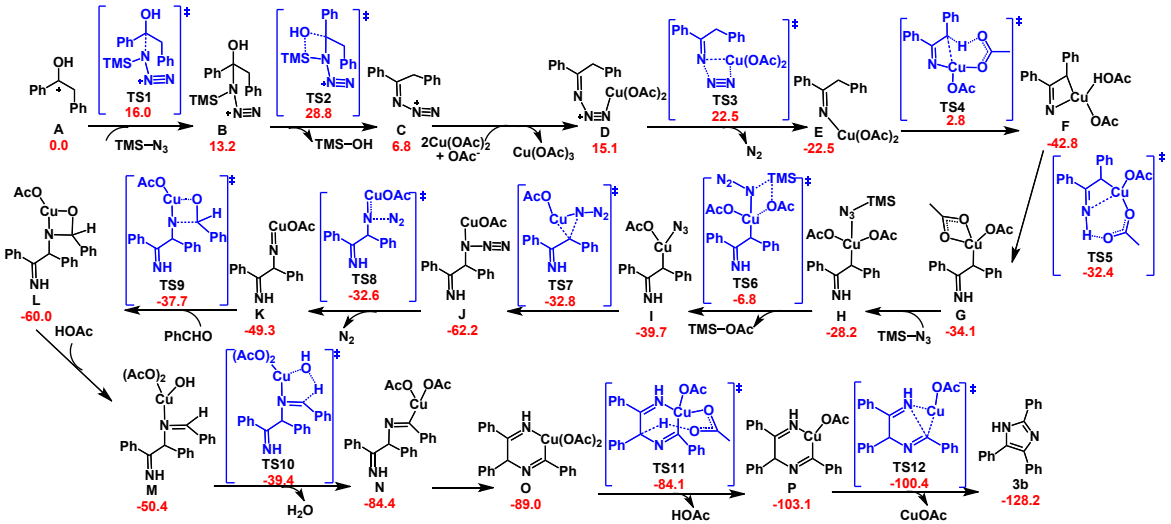



**Figure S1.** Free energy profile calculated for the copper-mediated C($sp^3$)-H azidation. The solvent-corrected free energies are given in kcal/mol.

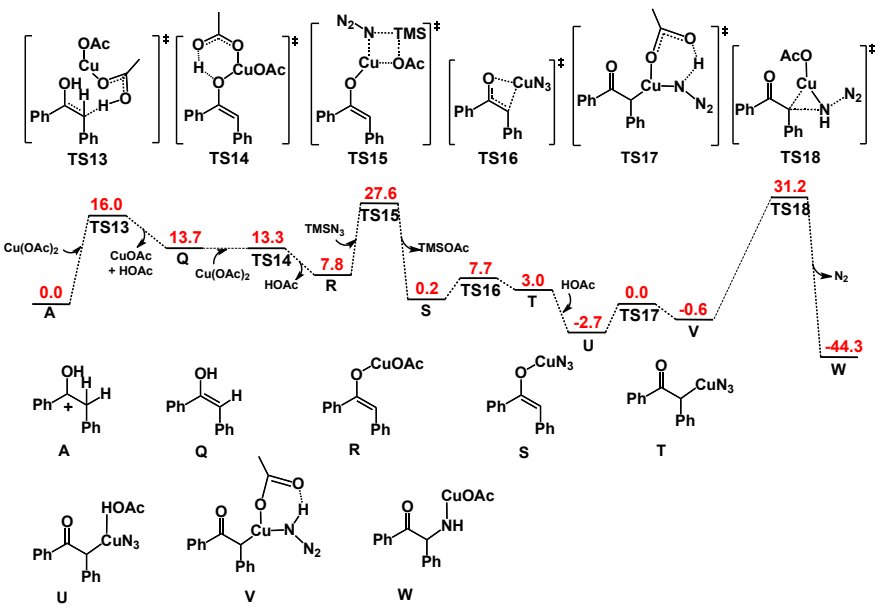


**Figure S2**. Free energy profile calculated for direct amination of the methylene group (**A** → **W**). The solvent-corrected free energies are given in kcal/mol.

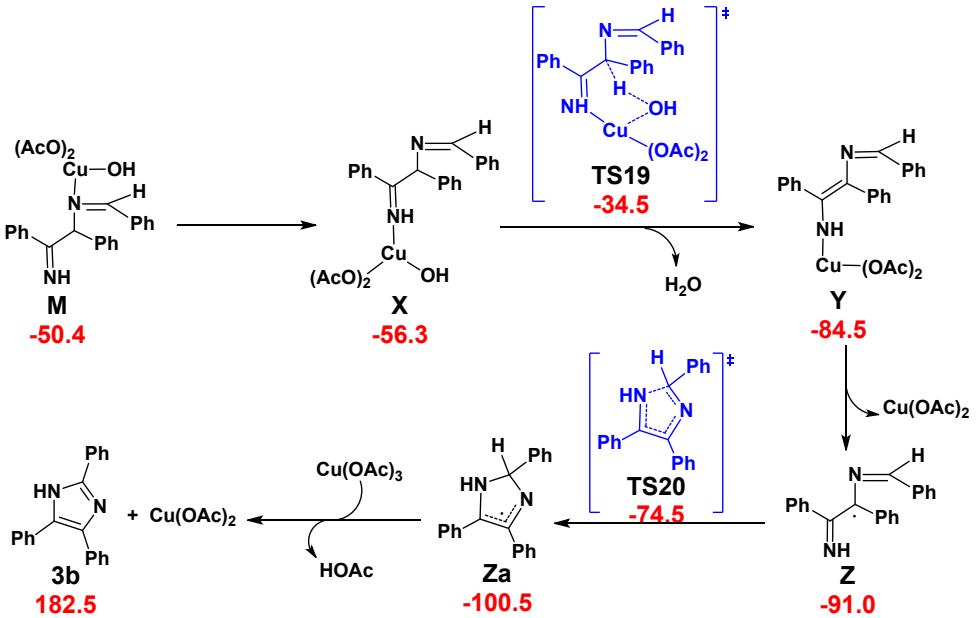



**Figure S3**. Alternative mechanism for transformation from **M** to final product. The solvent-corrected free energies are given in kcal/mol.

## (c) Cartesian Coordinates for All the Species Calculated in This Study

**AcOH**

E= -228.954076 a.u.

| | | | |
|---|---|---|---|
| 6 | -0.092709 | 0.124783 | 0.000053 |
| 8 | -0.654370 | 1.191813 | -0.000052 |
| 8 | -0.761313 | -1.047606 | -0.000031 |
| 1 | -1.706409 | -0.814063 | -0.000098 |
| 6 | 1.387434 | -0.098302 | 0.000049 |
| 1 | 1.679440 | -0.680795 | 0.881375 |
| 1 | 1.679427 | -0.680884 | -0.881223 |
| 1 | 1.904652 | 0.863204 | -0.000002 |

**$AcO^-$**

E= -228.3723691 a.u.

| | | | |
|---|---|---|---|
| 6 | -0.219557 | 0.000493 | -0.012686 |
| 8 | -0.763438 | -1.125388 | 0.002843 |
| 8 | -0.730372 | 1.142388 | 0.002840 |
| 6 | 1.344377 | -0.016080 | -0.004785 |
| 1 | 1.754789 | 0.830539 | -0.573682 |
| 1 | 1.703508 | 0.089051 | 1.031961 |
| 1 | 1.743263 | -0.962066 | -0.398917 |

**$Cu(OAc)_2$**

E= -652.9420509 a.u.

| | | | |
|---|---|---|---|
| 29 | -0.000028 | 0.000578 | -0.005999 |
| 8 | 1.657317 | 1.089317 | -0.003388 |
| 8 | -1.657669 | -1.084990 | -0.008776 |
| 6 | 2.319240 | 0.005209 | -0.002522 |
| 8 | 1.658697 | -1.081300 | -0.004454 |
| 6 | -2.319345 | 0.000251 | -0.008950 |
| 8 | -1.658412 | 1.085547 | -0.009364 |
| 6 | 3.807365 | -0.002634 | 0.016431 |
| 1 | 4.183997 | -0.702299 | -0.737077 |
| 1 | 4.203091 | 1.000644 | -0.160021 |
| 1 | 4.152021 | -0.362075 | 0.993435 |
| 6 | -3.807364 | -0.002636 | 0.019562 |
| 1 | -4.194813 | -0.867554 | -0.526779 |
| 1 | -4.142408 | -0.084790 | 1.060984 |
| 1 | -4.199904 | 0.929556 | -0.395845 |

**$Cu(OAc)_3$**

E= -881.2367561 a.u.

| | | | |
|---|---|---|---|
| 29 | 0.230779 | 0.024511 | -0.426525 |
| 8 | -0.938805 | -1.312454 | -0.850276 |
| 8 | 1.748672 | 1.167038 | -0.107867 |
| 6 | -1.160102 | -2.009661 | 0.250041 |
| 8 | -0.691139 | -1.729318 | 1.334530 |
| 6 | 2.465288 | 0.122136 | 0.029049 |
| 8 | 1.854779 | -0.979134 | -0.169498 |
| 6 | -2.080761 | -3.176666 | -0.015928 |
| 1 | -3.088035 | -2.802136 | -0.230372 |
| 1 | -1.745883 | -3.747015 | -0.888054 |
| 1 | -2.104807 | -3.813551 | 0.872461 |
| 6 | 3.899365 | 0.175642 | 0.386394 |
| 1 | 4.187860 | 1.196299 | 0.651841 |
| 1 | 4.092650 | -0.505600 | 1.222038 |
| 1 | 4.498418 | -0.166422 | -0.465900 |
| 6 | -1.408577 | 1.863318 | 0.271001 |
| 8 | -1.036609 | 1.273061 | -0.849014 |
| 8 | -1.013082 | 1.534915 | 1.371743 |
| 6 | -2.387675 | 2.982331 | 0.006001 |
| 1 | -3.314559 | 2.571713 | -0.409280 |
| 1 | -2.595791 | 3.496361 | 0.948200 |
| 1 | -1.978177 | 3.684078 | -0.728004 |

**CuOAc**

E= -424.5514659 a.u.

| | | | |
|---|---|---|---|
| 29 | -1.290123 | -0.002984 | 0.001942 |
| 6 | 1.052065 | 0.009075 | -0.007264 |

| | | | |
|---|---|---|---|
| 8 | 0.438087 | -1.100780 | -0.004838 |
| 8 | 0.434427 | 1.114516 | -0.004565 |
| 6 | 2.555486 | -0.001376 | 0.002669 |
| 1 | 2.926012 | -0.683168 | -0.770001 |
| 1 | 2.957646 | 1.002766 | -0.150620 |
| 1 | 2.904485 | -0.389127 | 0.967097 |

**$N_2$**

E= -109.4550063 a.u.

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 0.000000 | 0.552560 |
| 7 | 0.000000 | 0.000000 | -0.552560 |

**$TMSN_3$**

E= -573.2575537 a.u.

| | | | |
|---|---|---|---|
| 14 | -0.665605 | 0.000753 | 0.024219 |
| 6 | -0.656567 | -1.506469 | 1.136772 |
| 1 | -0.650871 | -2.435449 | 0.553485 |
| 1 | 0.235575 | -1.508440 | 1.778348 |
| 1 | -1.535618 | -1.524415 | 1.794379 |
| 6 | -0.657927 | 1.566488 | 1.052660 |
| 1 | 0.234252 | 1.604237 | 1.693066 |
| 1 | -0.653178 | 2.462390 | 0.419700 |
| 1 | -1.536953 | 1.619315 | 1.708416 |
| 6 | -2.033012 | -0.034760 | -1.243576 |
| 1 | -1.969390 | 0.834452 | -1.909610 |
| 1 | -1.966394 | -0.937545 | -1.863047 |
| 1 | -3.020910 | -0.023887 | -0.766118 |
| 7 | 0.831077 | -0.025404 | -0.943272 |
| 7 | 1.930526 | -0.011105 | -0.414027 |
| 7 | 2.990824 | 0.000400 | 0.011182 |

**TMSOAc**

E= -637.5332954 a.u.

| | | | |
|---|---|---|---|
| 14 | -0.979280 | 0.038054 | 0.000083 |
| 6 | -1.220433 | -0.967901 | -1.556706 |
| 1 | -0.981115 | -0.376953 | -2.450171 |
| 1 | -0.579833 | -1.856595 | -1.552375 |
| 1 | -2.265230 | -1.294597 | -1.645716 |
| 6 | -1.220304 | -0.967970 | 1.556837 |
| 1 | -0.579424 | -1.856467 | 1.552493 |
| 1 | -0.981315 | -0.377041 | 2.450397 |
| 1 | -2.264998 | -1.295053 | 1.645671 |
| 6 | -2.077573 | 1.551257 | -0.000101 |
| 1 | -1.896433 | 2.172751 | 0.885813 |
| 1 | -1.896752 | 2.172009 | -0.886611 |
| 1 | -3.138297 | 1.268004 | 0.000180 |
| 6 | 1.683660 | -0.039130 | -0.000063 |
| 8 | 1.636845 | -1.249223 | -0.000291 |
| 8 | 0.593026 | 0.738672 | 0.000128 |
| 6 | 2.949020 | 0.766354 | 0.000057 |
| 1 | 2.975669 | 1.418715 | -0.880561 |
| 1 | 2.975706 | 1.418331 | 0.880964 |
| 1 | 3.816751 | 0.102894 | -0.000090 |

**TMSOH**

E= -484.9538499 a.u.

| | | | |
|---|---|---|---|
| 14 | -0.005431 | 0.000005 | 0.045515 |
| 6 | 0.928075 | 1.526716 | -0.527893 |
| 1 | 0.407207 | 2.446247 | -0.232314 |
| 1 | 1.946472 | 1.572692 | -0.119356 |
| 1 | 1.017569 | 1.531484 | -1.623090 |
| 6 | 0.924822 | -1.529080 | -0.526830 |
| 1 | 1.943349 | -1.576608 | -0.118802 |
| 1 | 0.402298 | -2.447251 | -0.229941 |
| 1 | 1.013663 | -1.535231 | -1.622074 |
| 6 | -1.742320 | 0.001565 | -0.643811 |
| 1 | -2.298917 | -0.883701 | -0.312117 |
| 1 | -2.297046 | 0.888237 | -0.312747 |
| 1 | -1.731541 | 0.001146 | -1.741734 |
| 8 | -0.199839 | 0.000829 | 1.704672 |
| 1 | 0.608225 | 0.001089 | 2.228791 |

**$H_2O$**

E= -76.3738331 a.u.

| | | | |
|---|---|---|---|
| 8 | 0.000000 | 0.000000 | 0.118339 |
| 1 | 0.000000 | 0.760840 | -0.473357 |

| | | | |
|---|---|---|---|
| 1 | 0.000000 | -0.760840 | -0.473357 |

**PhCHO**

E= -345.316039 a.u.

| | | | |
|---|---|---|---|
| 6 | 1.982201 | 0.466463 | 0.000004 |
| 8 | 2.833338 | -0.394076 | -0.000005 |
| 1 | 2.257747 | 1.550441 | 0.000007 |
| 6 | 0.530705 | 0.214010 | 0.000002 |
| 6 | -0.359134 | 1.288495 | 0.000000 |
| 6 | 0.047799 | -1.097542 | 0.000003 |
| 6 | -1.729303 | 1.057225 | -0.000001 |
| 1 | 0.033030 | 2.306787 | 0.000000 |
| 6 | -1.319047 | -1.328220 | 0.000000 |
| 1 | 0.767362 | -1.914648 | 0.000004 |
| 6 | -2.206072 | -0.250766 | -0.000001 |
| 1 | -2.426153 | 1.893259 | -0.000003 |
| 1 | -1.702100 | -2.347095 | 0.000000 |
| 1 | -3.279489 | -0.434124 | -0.000003 |

**A**

E= -615.8128844 a.u.

| | | | |
|---|---|---|---|
| 6 | -0.545566 | 1.275903 | -0.499650 |
| 8 | -0.523147 | 2.481956 | -0.018861 |
| 6 | -1.583521 | 0.351909 | -0.159745 |
| 6 | -2.793916 | 0.802472 | 0.415178 |
| 6 | -1.414906 | -1.023448 | -0.426987 |
| 6 | -3.798346 | -0.097025 | 0.712418 |
| 1 | -2.991690 | 1.863796 | 0.571633 |
| 6 | -2.418727 | -1.918466 | -0.107913 |
| 1 | -0.474367 | -1.385878 | -0.835864 |
| 6 | -3.608219 | -1.457660 | 0.457013 |
| 1 | -4.737385 | 0.255206 | 1.131369 |
| 1 | -2.279224 | -2.979701 | -0.296933 |
| 1 | -4.400509 | -2.164225 | 0.695411 |
| 6 | 0.602910 | 0.989135 | -1.390832 |
| 1 | 0.962937 | 1.942359 | -1.799313 |
| 1 | 0.289881 | 0.351604 | -2.225130 |
| 6 | 1.687396 | 0.304008 | -0.567688 |
| 6 | 2.141579 | -0.965293 | -0.929367 |
| 6 | 2.241767 | 0.951661 | 0.537928 |
| 6 | 3.152126 | -1.576393 | -0.196127 |
| 1 | 1.731450 | -1.461391 | -1.810415 |
| 6 | 3.249270 | 0.334584 | 1.271129 |
| 1 | 1.906201 | 1.951550 | 0.814293 |
| 6 | 3.702421 | -0.929795 | 0.907415 |
| 1 | 3.518609 | -2.555871 | -0.495838 |
| 1 | 3.687030 | 0.846643 | 2.125224 |
| 1 | 4.493498 | -1.410185 | 1.478882 |
| 1 | -1.206878 | 2.640903 | 0.660927 |

**TS1**

E= -1189.0835774 a.u.

| | | | |
|---|---|---|---|
| 6 | 0.720392 | -0.459347 | 1.249064 |
| 8 | 0.399152 | -1.514349 | 1.972070 |
| 1 | 0.970189 | -2.274035 | 1.749480 |
| 6 | 1.958545 | -0.548735 | 0.459528 |
| 6 | 2.191925 | -1.679994 | -0.342704 |
| 6 | 2.964987 | 0.412880 | 0.598549 |
| 6 | 3.398977 | -1.828973 | -1.004630 |
| 1 | 1.401774 | -2.418741 | -0.491220 |
| 6 | 4.178963 | 0.250137 | -0.058655 |
| 1 | 2.830434 | 1.263715 | 1.260699 |
| 6 | 4.395025 | -0.862658 | -0.862923 |
| 1 | 3.565317 | -2.695881 | -1.639545 |
| 1 | 4.960261 | 0.995961 | 0.066703 |
| 1 | 5.344225 | -0.982239 | -1.380538 |
| 7 | -0.666248 | -0.741133 | -0.267888 |
| 7 | -0.403204 | -0.107399 | -1.293626 |
| 7 | -0.085947 | 0.498854 | -2.199119 |
| 6 | 0.175778 | 0.812140 | 1.841756 |
| 1 | 0.970780 | 1.166453 | 2.521653 |
| 1 | -0.648873 | 0.506293 | 2.498634 |
| 6 | -0.279899 | 1.920598 | 0.921780 |
| 6 | 0.598681 | 2.844808 | 0.356395 |
| 6 | -1.645996 | 2.045675 | 0.650083 |
| 6 | 0.128599 | 3.845193 | -0.489706 |

| | | | |
|---|---|---|---|
| 1 | 1.663083 | 2.806448 | 0.580274 |
| 6 | -2.118112 | 3.038307 | -0.199572 |
| 1 | -2.349653 | 1.354923 | 1.117270 |
| 6 | -1.227571 | 3.938315 | -0.778327 |
| 1 | 0.829132 | 4.558288 | -0.919029 |
| 1 | -3.185500 | 3.119852 | -0.396581 |
| 1 | -1.593232 | 4.719940 | -1.440704 |
| 14 | -2.209457 | -1.751882 | -0.181963 |
| 6 | -2.941068 | -1.483381 | 1.509858 |
| 1 | -3.753688 | -2.207008 | 1.661320 |
| 1 | -2.212701 | -1.643221 | 2.313734 |
| 1 | -3.377296 | -0.483476 | 1.625036 |
| 6 | -3.267487 | -1.092832 | -1.567294 |
| 1 | -3.433775 | -0.011886 | -1.460499 |
| 1 | -2.824325 | -1.272969 | -2.555308 |
| 1 | -4.251390 | -1.578869 | -1.559114 |
| 6 | -1.643758 | -3.511566 | -0.442896 |
| 1 | -2.506127 | -4.190696 | -0.470122 |
| 1 | -1.109915 | -3.626164 | -1.395376 |
| 1 | -0.989608 | -3.861203 | 0.366747 |

**B**

E= -1189.0907225 a.u.

| | | | |
|---|---|---|---|
| 6 | 0.428673 | 0.589303 | -0.946151 |
| 8 | 0.132163 | 1.692563 | -1.716242 |
| 1 | 0.718680 | 2.425431 | -1.463415 |
| 6 | 1.799770 | 0.694610 | -0.319257 |
| 6 | 2.004219 | 1.568534 | 0.756481 |
| 6 | 2.903989 | 0.061931 | -0.895487 |
| 6 | 3.279024 | 1.771708 | 1.270241 |
| 1 | 1.159903 | 2.096244 | 1.203506 |
| 6 | 4.178986 | 0.269292 | -0.380913 |
| 1 | 2.785920 | -0.588789 | -1.759181 |
| 6 | 4.368733 | 1.116614 | 0.705404 |
| 1 | 3.420423 | 2.445294 | 2.112473 |
| 1 | 5.028703 | -0.233105 | -0.837771 |
| 1 | 5.366882 | 1.271437 | 1.109039 |
| 7 | -0.654432 | 0.665868 | 0.220267 |
| 7 | -0.479331 | -0.095443 | 1.203453 |
| 7 | -0.326474 | -0.735735 | 2.118913 |
| 6 | 0.082441 | -0.660884 | -1.758859 |
| 1 | 0.878194 | -0.795776 | -2.503339 |
| 1 | -0.817256 | -0.402296 | -2.333734 |
| 6 | -0.162609 | -1.901967 | -0.944455 |
| 6 | 0.883300 | -2.656442 | -0.406982 |
| 6 | -1.478495 | -2.281614 | -0.657020 |
| 6 | 0.619322 | -3.737316 | 0.427505 |
| 1 | 1.916873 | -2.396214 | -0.631518 |
| 6 | -1.746067 | -3.359012 | 0.180105 |
| 1 | -2.305173 | -1.728210 | -1.107817 |
| 6 | -0.694002 | -4.082534 | 0.734285 |
| 1 | 1.444544 | -4.313485 | 0.840843 |
| 1 | -2.775867 | -3.641122 | 0.391125 |
| 1 | -0.897755 | -4.925578 | 1.390997 |
| 14 | -2.284359 | 1.645479 | 0.130952 |
| 6 | -3.029398 | 1.323147 | -1.537861 |
| 1 | -3.956504 | 1.907333 | -1.620914 |
| 1 | -2.364831 | 1.635156 | -2.350522 |
| 1 | -3.300422 | 0.269531 | -1.678352 |
| 6 | -3.241930 | 0.875102 | 1.530678 |
| 1 | -3.367536 | -0.209029 | 1.403251 |
| 1 | -2.800106 | 1.062344 | 2.517780 |
| 1 | -4.249287 | 1.312100 | 1.547706 |
| 6 | -1.796061 | 3.411191 | 0.454935 |
| 1 | -2.700777 | 4.015492 | 0.606609 |
| 1 | -1.192674 | 3.505797 | 1.367082 |
| 1 | -1.245920 | 3.857422 | -0.381558 |

**TS2**

E= -1189.0637073 a.u.

| | | | |
|---|---|---|---|
| 6 | 0.276691 | -0.220149 | -0.689273 |
| 8 | 1.585842 | -0.020123 | -1.298426 |
| 1 | 2.028731 | -0.880682 | -1.415391 |
| 6 | 0.149967 | -1.665069 | -0.269097 |
| 6 | 0.833399 | -2.111875 | 0.870104 |
| 6 | -0.528827 | -2.596940 | -1.059943 |

| | | | |
|---|---|---|---|
| 6 | 0.813358 | -3.454412 | 1.224777 |
| 1 | 1.381908 | -1.405950 | 1.495837 |
| 6 | -0.547091 | -3.940720 | -0.701715 |
| 1 | -1.050105 | -2.289303 | -1.963764 |
| 6 | 0.118196 | -4.370985 | 0.440937 |
| 1 | 1.339884 | -3.784686 | 2.117429 |
| 1 | -1.085598 | -4.653139 | -1.322513 |
| 1 | 0.098754 | -5.422110 | 0.719997 |
| 7 | 0.516297 | 0.703172 | 0.445646 |
| 7 | -0.263128 | 0.726356 | 1.412225 |
| 7 | -0.889291 | 0.808692 | 2.351349 |
| 6 | -0.780345 | 0.369290 | -1.619504 |
| 1 | -0.954528 | -0.323553 | -2.452759 |
| 1 | -0.327845 | 1.268687 | -2.059360 |
| 6 | -2.048724 | 0.740259 | -0.896989 |
| 6 | -2.973227 | -0.221576 | -0.481380 |
| 6 | -2.280075 | 2.081113 | -0.577253 |
| 6 | -4.095036 | 0.150008 | 0.251369 |
| 1 | -2.817951 | -1.272002 | -0.725962 |
| 6 | -3.403032 | 2.455057 | 0.151806 |
| 1 | -1.570464 | 2.840269 | -0.911464 |
| 6 | -4.309627 | 1.487074 | 0.573565 |
| 1 | -4.807221 | -0.608448 | 0.569874 |
| 1 | -3.573074 | 3.503637 | 0.387691 |
| 1 | -5.188645 | 1.775243 | 1.146292 |
| 14 | 2.653567 | 1.349771 | -0.028226 |
| 6 | 2.198222 | 2.860996 | -0.999822 |
| 1 | 2.993532 | 3.610593 | -0.886553 |
| 1 | 2.094591 | 2.641756 | -2.068652 |
| 1 | 1.266492 | 3.310423 | -0.636319 |
| 6 | 2.817923 | 1.599812 | 1.816879 |
| 1 | 2.045741 | 2.263723 | 2.224147 |
| 1 | 2.792078 | 0.653110 | 2.373413 |
| 1 | 3.797791 | 2.056411 | 2.017110 |
| 6 | 4.186084 | 0.432072 | -0.579491 |
| 1 | 5.068418 | 0.996464 | -0.247037 |
| 1 | 4.260150 | -0.558022 | -0.106943 |
| 1 | 4.256415 | 0.310486 | -1.666863 |

**C**

E= -704.1067217 a.u.

| | | | |
|---|---|---|---|
| 6 | -0.385390 | 0.503659 | 0.740638 |
| 6 | -1.616975 | -0.110764 | 0.339346 |
| 6 | -2.757544 | 0.656394 | -0.000720 |
| 6 | -1.719713 | -1.522460 | 0.321590 |
| 6 | -3.935212 | 0.034717 | -0.364250 |
| 1 | -2.753366 | 1.739696 | 0.089605 |
| 6 | -2.893255 | -2.135026 | -0.074859 |
| 1 | -0.864597 | -2.139509 | 0.585080 |
| 6 | -4.000791 | -1.359703 | -0.417765 |
| 1 | -4.812900 | 0.631816 | -0.598084 |
| 1 | -2.953044 | -3.219695 | -0.109386 |
| 1 | -4.928637 | -1.844524 | -0.714246 |
| 7 | -0.021151 | 1.773209 | 0.468458 |
| 7 | -0.590782 | 2.475703 | -0.408371 |
| 7 | -0.916570 | 3.247498 | -1.162265 |
| 6 | 0.670913 | -0.193359 | 1.530019 |
| 1 | 0.299266 | -1.135233 | 1.943649 |
| 1 | 0.924692 | 0.454524 | 2.381657 |
| 6 | 1.895697 | -0.377938 | 0.650871 |
| 6 | 1.902965 | -1.349810 | -0.351854 |
| 6 | 3.006365 | 0.449928 | 0.818680 |
| 6 | 3.023913 | -1.514389 | -1.157804 |
| 1 | 1.037623 | -1.996425 | -0.502112 |
| 6 | 4.125577 | 0.284155 | 0.012077 |
| 1 | 3.000206 | 1.214203 | 1.595735 |
| 6 | 4.135418 | -0.697146 | -0.976492 |
| 1 | 3.028886 | -2.282533 | -1.928008 |
| 1 | 4.996557 | 0.918659 | 0.160700 |
| 1 | 5.013034 | -0.825404 | -1.606197 |

**D**

E= -1357.299476 a.u.

| | | | |
|---|---|---|---|
| 6 | 1.045773 | -0.891195 | 1.173535 |
| 6 | 1.373587 | -1.959635 | 0.222383 |
| 6 | 0.422089 | -2.362507 | -0.728485 |

| | | | |
|---|---|---|---|
| 6 | 2.632203 | -2.575507 | 0.237735 |
| 6 | 0.721547 | -3.376913 | -1.624382 |
| 1 | -0.541311 | -1.856637 | -0.772697 |
| 6 | 2.921585 | -3.595971 | -0.655968 |
| 1 | 3.391133 | -2.262750 | 0.952174 |
| 6 | 1.967354 | -3.999161 | -1.586206 |
| 1 | -0.018272 | -3.676381 | -2.363620 |
| 1 | 3.898020 | -4.075279 | -0.630233 |
| 1 | 2.199732 | -4.794198 | -2.292540 |
| 7 | -0.220302 | -0.647787 | 1.306504 |
| 6 | 2.136688 | -0.124268 | 1.863942 |
| 1 | 2.757913 | -0.834698 | 2.428827 |
| 1 | 1.679111 | 0.545343 | 2.605123 |
| 6 | 2.999701 | 0.653715 | 0.898075 |
| 6 | 4.383171 | 0.685988 | 1.070295 |
| 6 | 2.421000 | 1.364107 | -0.156594 |
| 6 | 5.184464 | 1.428717 | 0.210018 |
| 1 | 4.836804 | 0.127085 | 1.890803 |
| 6 | 3.227017 | 2.098022 | -1.020493 |
| 1 | 1.337860 | 1.340155 | -0.315332 |
| 6 | 4.606519 | 2.136271 | -0.839082 |
| 1 | 6.262939 | 1.449954 | 0.357323 |
| 1 | 2.769924 | 2.641932 | -1.846112 |
| 1 | 5.231292 | 2.715813 | -1.516481 |
| 29 | -2.329189 | 0.591712 | 0.170144 |
| 6 | -4.052226 | -1.004629 | -0.030458 |
| 8 | -3.661912 | -0.459982 | 1.067463 |
| 8 | -3.473726 | -0.710917 | -1.101985 |
| 6 | -1.351421 | 2.562947 | -1.037654 |
| 8 | -2.490742 | 2.902930 | -0.729354 |
| 8 | -0.860231 | 1.395483 | -0.725913 |
| 6 | -5.203690 | -1.956392 | 0.025629 |
| 1 | -5.347293 | -2.441051 | -0.943730 |
| 1 | -5.036011 | -2.706170 | 0.806571 |
| 1 | -6.112568 | -1.405067 | 0.294789 |
| 6 | -0.400553 | 3.456393 | -1.791173 |
| 1 | 0.464160 | 3.687996 | -1.155097 |
| 1 | -0.024003 | 2.938442 | -2.681388 |
| 1 | -0.900043 | 4.384241 | -2.081062 |
| 7 | -0.555038 | 0.449400 | 2.091499 |
| 7 | -1.455929 | 1.170048 | 1.867727 |

**TS3**

E= -1357.2863335 a.u.

| | | | |
|---|---|---|---|
| 6 | -0.881146 | 0.761026 | 1.265179 |
| 6 | -1.145018 | 1.769914 | 0.199422 |
| 6 | -0.410187 | 1.733623 | -0.989223 |
| 6 | -2.114520 | 2.757172 | 0.404139 |
| 6 | -0.652967 | 2.687455 | -1.970609 |
| 1 | 0.319587 | 0.942442 | -1.151705 |
| 6 | -2.342333 | 3.707867 | -0.580288 |
| 1 | -2.686474 | 2.787464 | 1.330835 |
| 6 | -1.610859 | 3.674826 | -1.766329 |
| 1 | -0.084850 | 2.655367 | -2.897909 |
| 1 | -3.096659 | 4.476724 | -0.424090 |
| 1 | -1.793434 | 4.422845 | -2.535891 |
| 7 | 0.347312 | 0.570562 | 1.492417 |
| 6 | -2.047269 | 0.093138 | 1.962279 |
| 1 | -2.557204 | 0.862930 | 2.560950 |
| 1 | -1.645496 | -0.643906 | 2.668277 |
| 6 | -3.006856 | -0.526470 | 0.983982 |
| 6 | -4.360194 | -0.192811 | 1.010902 |
| 6 | -2.544413 | -1.448709 | 0.040239 |
| 6 | -5.250596 | -0.782997 | 0.120326 |
| 1 | -4.721077 | 0.534011 | 1.740462 |
| 6 | -3.435144 | -2.030794 | -0.853822 |
| 1 | -1.479462 | -1.692549 | -0.009957 |
| 6 | -4.788172 | -1.703883 | -0.813848 |
| 1 | -6.306170 | -0.518890 | 0.153743 |
| 1 | -3.069432 | -2.746203 | -1.588809 |
| 1 | -5.482073 | -2.164413 | -1.515007 |
| 29 | 2.190469 | -0.594025 | 0.214022 |
| 6 | 3.825108 | 1.106413 | -0.001612 |
| 8 | 3.599678 | 0.390805 | 1.042943 |
| 8 | 3.123147 | 0.935335 | -1.024283 |
| 6 | 1.309941 | -2.436995 | -1.241877 |

| | | | |
|---|---|---|---|
| 8 | 2.512184 | -2.658487 | -1.112466 |
| 8 | 0.727894 | -1.422190 | -0.665417 |
| 6 | 4.945049 | 2.094471 | 0.044071 |
| 1 | 5.006348 | 2.560437 | 1.032700 |
| 1 | 5.890874 | 1.568519 | -0.135674 |
| 1 | 4.815252 | 2.853022 | -0.733153 |
| 6 | 0.391882 | -3.317373 | -2.046295 |
| 1 | -0.235865 | -3.905825 | -1.364072 |
| 1 | -0.273668 | -2.708379 | -2.668908 |
| 1 | 0.974333 | -4.001243 | -2.669465 |
| 7 | 0.681268 | -0.967711 | 2.455519 |
| 7 | 1.529248 | -1.559219 | 1.977065 |

**E**

E= -1247.8888327 a.u.

| | | | |
|---|---|---|---|
| 6 | -0.764566 | 0.193512 | 1.141778 |
| 6 | -0.693159 | 1.161008 | 0.017853 |
| 6 | -0.488246 | 0.683948 | -1.276249 |
| 6 | -0.845085 | 2.527844 | 0.252793 |
| 6 | -0.430508 | 1.580043 | -2.336687 |
| 1 | -0.370830 | -0.387467 | -1.442677 |
| 6 | -0.755550 | 3.419366 | -0.809660 |
| 1 | -1.000395 | 2.895115 | 1.267781 |
| 6 | -0.553224 | 2.944905 | -2.103450 |
| 1 | -0.270400 | 1.208588 | -3.346596 |
| 1 | -0.849300 | 4.488627 | -0.627942 |
| 1 | -0.489837 | 3.646178 | -2.933468 |
| 7 | 0.126585 | -0.624715 | 1.485876 |
| 6 | -2.091080 | 0.106106 | 1.899576 |
| 1 | -2.346697 | 1.117842 | 2.246943 |
| 1 | -1.948714 | -0.534898 | 2.777555 |
| 6 | -3.147660 | -0.433471 | 0.976020 |
| 6 | -4.117563 | 0.401896 | 0.422942 |
| 6 | -3.127252 | -1.784755 | 0.624018 |
| 6 | -5.069962 | -0.110535 | -0.451890 |
| 1 | -4.123001 | 1.461568 | 0.681558 |
| 6 | -4.077107 | -2.297069 | -0.250699 |
| 1 | -2.352022 | -2.431447 | 1.038215 |
| 6 | -5.052370 | -1.460206 | -0.788243 |
| 1 | -5.826457 | 0.548836 | -0.874057 |
| 1 | -4.055806 | -3.352566 | -0.516249 |
| 1 | -5.796347 | -1.860701 | -1.474865 |
| 29 | 1.758405 | -0.723931 | 0.608358 |
| 6 | 2.586491 | 1.654984 | 0.379794 |
| 8 | 2.250804 | 0.895137 | 1.392303 |
| 8 | 2.490145 | 1.302584 | -0.789160 |
| 6 | 2.659975 | -2.439968 | -0.672537 |
| 8 | 3.434321 | -1.607117 | -0.133392 |
| 8 | 1.402971 | -2.324785 | -0.440609 |
| 6 | 3.080415 | 3.016547 | 0.797825 |
| 1 | 3.382743 | 3.586700 | -0.084764 |
| 1 | 2.279800 | 3.547845 | 1.326440 |
| 1 | 3.922174 | 2.919092 | 1.492110 |
| 6 | 3.148764 | -3.530444 | -1.562440 |
| 1 | 2.790769 | -4.497865 | -1.192768 |
| 1 | 2.733971 | -3.392189 | -2.567795 |
| 1 | 4.240688 | -3.525053 | -1.610533 |

**TS4**

E= -1247.8431139 a.u.

| | | | |
|---|---|---|---|
| 6 | -1.262668 | -0.592803 | 0.570764 |
| 6 | -2.732015 | -0.551937 | 0.507207 |
| 6 | -3.448719 | -1.751920 | 0.436964 |
| 6 | -3.413645 | 0.667206 | 0.521205 |
| 6 | -4.833536 | -1.729029 | 0.388662 |
| 1 | -2.901374 | -2.693327 | 0.427168 |
| 6 | -4.802455 | 0.684027 | 0.468565 |
| 1 | -2.859828 | 1.604985 | 0.555608 |
| 6 | -5.512025 | -0.510941 | 0.404894 |
| 1 | -5.389864 | -2.663158 | 0.340478 |
| 1 | -5.331591 | 1.634947 | 0.474750 |
| 1 | -6.599749 | -0.494433 | 0.366134 |
| 7 | -0.564568 | -1.647882 | 0.457832 |
| 6 | -0.409063 | 0.635804 | 0.818598 |
| 1 | -0.837263 | 1.108551 | 1.719912 |
| 6 | -0.247069 | 1.585397 | -0.322151 |

| | | | |
|---|---|---|---|
| 6 | -0.429630 | 1.179477 | -1.647180 |
| 6 | 0.113404 | 2.911628 | -0.053174 |
| 6 | -0.270025 | 2.092220 | -2.682879 |
| 1 | -0.665461 | 0.140201 | -1.872794 |
| 6 | 0.262880 | 3.820602 | -1.091936 |
| 1 | 0.281216 | 3.221540 | 0.978859 |
| 6 | 0.070742 | 3.413042 | -2.410038 |
| 1 | -0.407194 | 1.763313 | -3.711041 |
| 1 | 0.533804 | 4.851838 | -0.871522 |
| 1 | 0.195068 | 4.125248 | -3.223864 |
| 29 | 1.143756 | -0.890864 | 0.515021 |
| 6 | 2.797169 | 0.963078 | 1.600265 |
| 8 | 2.807126 | 0.056377 | 0.713538 |
| 8 | 1.769003 | 1.293835 | 2.250960 |
| 6 | 1.991113 | -2.414318 | -1.257705 |
| 8 | 1.503940 | -1.446895 | -1.849275 |
| 8 | 1.988001 | -2.533650 | 0.030541 |
| 6 | 4.095697 | 1.672906 | 1.859130 |
| 1 | 4.015968 | 2.333558 | 2.725691 |
| 1 | 4.891442 | 0.936249 | 2.010048 |
| 1 | 4.361942 | 2.259412 | 0.971872 |
| 6 | 2.658012 | -3.556540 | -1.985410 |
| 1 | 2.258188 | -4.513309 | -1.633325 |
| 1 | 2.505563 | -3.452282 | -3.062788 |
| 1 | 3.731531 | -3.549057 | -1.764219 |
| 1 | 0.687100 | 0.691221 | 1.507802 |

**F**

E= -1247.9193253 a.u.

| | | | |
|---|---|---|---|
| 6 | 1.688171 | -0.725053 | 0.127559 |
| 6 | 3.130866 | -0.918088 | 0.101905 |
| 6 | 3.740093 | -1.747305 | 1.049205 |
| 6 | 3.901672 | -0.277084 | -0.870062 |
| 6 | 5.113516 | -1.933206 | 1.018551 |
| 1 | 3.117210 | -2.236002 | 1.797604 |
| 6 | 5.277893 | -0.466190 | -0.897207 |
| 1 | 3.412719 | 0.371862 | -1.597411 |
| 6 | 5.881912 | -1.293587 | 0.045696 |
| 1 | 5.591600 | -2.579302 | 1.752458 |
| 1 | 5.881052 | 0.032555 | -1.653424 |
| 1 | 6.960333 | -1.441759 | 0.023932 |
| 7 | 0.788978 | -1.180097 | 0.901953 |
| 6 | 0.756833 | 0.050101 | -0.683818 |
| 1 | 0.343202 | -0.446343 | -1.565608 |
| 6 | 0.606161 | 1.496793 | -0.575818 |
| 6 | 1.387476 | 2.258228 | 0.305619 |
| 6 | -0.343935 | 2.142137 | -1.383074 |
| 6 | 1.231549 | 3.635114 | 0.362033 |
| 1 | 2.115910 | 1.761629 | 0.946953 |
| 6 | -0.487647 | 3.519246 | -1.328872 |
| 1 | -0.981436 | 1.536378 | -2.027766 |
| 6 | 0.299386 | 4.268896 | -0.457135 |
| 1 | 1.841535 | 4.220590 | 1.047610 |
| 1 | -1.227645 | 4.011465 | -1.956966 |
| 1 | 0.180051 | 5.349822 | -0.408995 |
| 29 | -0.940109 | -0.474502 | 0.440351 |
| 6 | -3.087360 | -1.642425 | -1.536028 |
| 8 | -2.076896 | -0.952730 | -1.433017 |
| 8 | -3.773870 | -2.114159 | -0.523028 |
| 6 | -2.981982 | 0.186229 | 1.692259 |
| 8 | -2.286853 | 1.069191 | 1.147538 |
| 8 | -2.666287 | -1.055928 | 1.610440 |
| 6 | -3.658923 | -2.043846 | -2.861042 |
| 1 | -3.597558 | -3.133282 | -2.968979 |
| 1 | -4.720345 | -1.776594 | -2.906720 |
| 1 | -3.111538 | -1.561630 | -3.673728 |
| 6 | -4.227283 | 0.541469 | 2.456705 |
| 1 | -5.095846 | 0.073655 | 1.975783 |
| 1 | -4.166706 | 0.130403 | 3.470872 |
| 1 | -4.370186 | 1.624291 | 2.498873 |
| 1 | -3.371157 | -1.796049 | 0.347336 |

**TS5**

E= -1247.9003486 a.u.

| | | | |
|---|---|---|---|
| 6 | 0.989752 | -0.765172 | -0.877401 |
| 6 | 2.308771 | -1.062325 | -0.313168 |

| | | | |
|---|---|---|---|
| 6 | 2.494217 | -2.227584 | 0.439494 |
| 6 | 3.390688 | -0.211023 | -0.560335 |
| 6 | 3.752345 | -2.533522 | 0.938552 |
| 1 | 1.643598 | -2.877972 | 0.641731 |
| 6 | 4.649252 | -0.526957 | -0.068130 |
| 1 | 3.237432 | 0.696083 | -1.144366 |
| 6 | 4.829007 | -1.687101 | 0.681830 |
| 1 | 3.895530 | -3.434789 | 1.531113 |
| 1 | 5.492338 | 0.131280 | -0.268219 |
| 1 | 5.815456 | -1.931918 | 1.071991 |
| 7 | 0.026165 | -1.603368 | -1.079115 |
| 6 | 0.453622 | 0.558018 | -1.256151 |
| 1 | 0.151780 | 0.622965 | -2.304938 |
| 6 | 0.626447 | 1.808203 | -0.553764 |
| 6 | 1.091978 | 1.874881 | 0.770782 |
| 6 | 0.259782 | 2.997986 | -1.206987 |
| 6 | 1.227147 | 3.100069 | 1.401531 |
| 1 | 1.314635 | 0.956285 | 1.310167 |
| 6 | 0.402242 | 4.222310 | -0.574587 |
| 1 | -0.147438 | 2.941629 | -2.216348 |
| 6 | 0.889105 | 4.274829 | 0.730752 |
| 1 | 1.580484 | 3.140945 | 2.429558 |
| 1 | 0.123970 | 5.137596 | -1.093258 |
| 1 | 0.993457 | 5.235611 | 1.232042 |
| 29 | -1.364252 | -0.383676 | -0.753494 |
| 6 | -2.270486 | -2.927808 | 0.243126 |
| 8 | -2.636814 | -1.784648 | -0.153874 |
| 8 | -1.100772 | -3.409524 | 0.160333 |
| 6 | -2.304984 | 1.445366 | 0.675420 |
| 8 | -2.417532 | 1.179888 | -0.587822 |
| 8 | -1.602737 | 0.776912 | 1.442215 |
| 6 | -3.331898 | -3.781569 | 0.883687 |
| 1 | -4.228148 | -3.792587 | 0.254318 |
| 1 | -2.969726 | -4.799359 | 1.050951 |
| 1 | -3.617039 | -3.332099 | 1.842454 |
| 6 | -3.075852 | 2.653322 | 1.142330 |
| 1 | -2.911355 | 2.822566 | 2.209885 |
| 1 | -2.760407 | 3.535677 | 0.571893 |
| 1 | -4.145278 | 2.510592 | 0.948176 |
| 1 | -0.313111 | -2.584889 | -0.530712 |

**G**

E= -1247.9034661 a.u.

| | | | |
|---|---|---|---|
| 6 | 0.768853 | -0.430847 | -1.467702 |
| 6 | -0.171723 | 0.648020 | -1.068984 |
| 6 | 2.180887 | -0.489435 | -1.010141 |
| 6 | 3.051602 | 0.584454 | -1.218333 |
| 6 | 2.669995 | -1.673022 | -0.449767 |
| 6 | 4.389838 | 0.478398 | -0.859181 |
| 1 | 2.680314 | 1.503678 | -1.671223 |
| 6 | 4.004509 | -1.766705 | -0.070341 |
| 1 | 1.983604 | -2.505798 | -0.290961 |
| 6 | 4.865896 | -0.693236 | -0.276163 |
| 1 | 5.064608 | 1.314411 | -1.034392 |
| 1 | 4.372705 | -2.685290 | 0.383548 |
| 1 | 5.911995 | -0.769517 | 0.015341 |
| 6 | 0.062435 | 1.821418 | -0.255234 |
| 6 | 1.011508 | 1.897272 | 0.786470 |
| 6 | -0.764533 | 2.939530 | -0.498464 |
| 6 | 1.148905 | 3.065624 | 1.516402 |
| 1 | 1.606805 | 1.023918 | 1.032484 |
| 6 | -0.618294 | 4.104741 | 0.233987 |
| 1 | -1.526323 | 2.867158 | -1.274834 |
| 6 | 0.344829 | 4.171172 | 1.240075 |
| 1 | 1.882472 | 3.115102 | 2.318528 |
| 1 | -1.256064 | 4.961543 | 0.026985 |
| 1 | 0.460992 | 5.085105 | 1.820143 |
| 29 | -1.495222 | -0.425156 | 0.064297 |
| 6 | -3.823675 | -0.567434 | -0.295243 |
| 8 | -3.405240 | -1.100075 | 0.755772 |
| 8 | -2.989031 | 0.046589 | -1.061386 |
| 6 | -5.255536 | -0.639895 | -0.716325 |
| 1 | -5.584994 | 0.322425 | -1.121853 |
| 1 | -5.354268 | -1.385352 | -1.514963 |
| 1 | -5.885390 | -0.938261 | 0.126085 |
| 1 | -0.931843 | 0.782821 | -1.845026 |

| | | | |
|---|---|---|---|
| 7 | 0.249429 | -1.298839 | -2.258306 |
| 1 | 0.933852 | -2.026208 | -2.486733 |
| 6 | 0.062045 | -1.984543 | 1.424379 |
| 8 | -0.379873 | -2.791931 | 0.613226 |
| 8 | -0.175026 | -0.702344 | 1.360763 |
| 6 | 0.958138 | -2.377581 | 2.572315 |
| 1 | 1.888050 | -1.795533 | 2.536973 |
| 1 | 0.465273 | -2.147190 | 3.524058 |
| 1 | 1.182925 | -3.447094 | 2.525851 |

**H**

E= -1821.185527 a.u.

| | | | |
|---|---|---|---|
| 6 | 1.721635 | -0.339567 | -1.450056 |
| 6 | 1.237403 | 1.010489 | -1.038305 |
| 6 | 3.003938 | -0.904395 | -0.964772 |
| 6 | 4.181579 | -0.150656 | -0.976989 |
| 6 | 3.042166 | -2.236529 | -0.538794 |
| 6 | 5.380947 | -0.723327 | -0.572100 |
| 1 | 4.159723 | 0.885900 | -1.312852 |
| 6 | 4.240806 | -2.797724 | -0.113162 |
| 1 | 2.116132 | -2.813021 | -0.506431 |
| 6 | 5.410729 | -2.044525 | -0.132847 |
| 1 | 6.296142 | -0.134451 | -0.595357 |
| 1 | 4.259031 | -3.828640 | 0.235779 |
| 1 | 6.349486 | -2.486531 | 0.196857 |
| 6 | 1.701071 | 1.848501 | 0.039061 |
| 6 | 2.383338 | 1.380211 | 1.182322 |
| 6 | 1.400962 | 3.224711 | -0.051475 |
| 6 | 2.772672 | 2.267693 | 2.170964 |
| 1 | 2.589711 | 0.319802 | 1.286968 |
| 6 | 1.789968 | 4.104769 | 0.941582 |
| 1 | 0.845928 | 3.580277 | -0.919484 |
| 6 | 2.480804 | 3.626376 | 2.054895 |
| 1 | 3.301717 | 1.898999 | 3.047452 |
| 1 | 1.553046 | 5.163149 | 0.856236 |
| 1 | 2.788740 | 4.315630 | 2.839424 |
| 29 | -0.628363 | 0.310953 | -0.482517 |
| 6 | -2.200137 | 2.269654 | -1.057852 |
| 8 | -2.326676 | 2.183424 | 0.167728 |
| 8 | -1.350505 | 1.573909 | -1.742301 |
| 6 | -3.077831 | 3.181141 | -1.880253 |
| 1 | -3.524632 | 3.951945 | -1.245507 |
| 1 | -2.517671 | 3.635888 | -2.703718 |
| 1 | -3.883494 | 2.582292 | -2.324954 |
| 7 | -2.436780 | -0.829648 | -0.459054 |
| 7 | -2.430009 | -1.727756 | -1.298808 |
| 7 | -2.395961 | -2.530551 | -2.101605 |
| 1 | 0.816901 | 1.555257 | -1.886393 |
| 7 | 0.921340 | -0.953789 | -2.243594 |
| 1 | 1.275451 | -1.886591 | -2.474140 |
| 14 | -3.584095 | -0.919362 | 0.944327 |
| 6 | -2.717074 | -0.151506 | 2.399216 |
| 1 | -1.778885 | -0.668068 | 2.632497 |
| 1 | -2.474540 | 0.891983 | 2.164335 |
| 1 | -3.365051 | -0.175957 | 3.285546 |
| 6 | -5.097108 | 0.049826 | 0.430264 |
| 1 | -4.799800 | 1.086707 | 0.226119 |
| 1 | -5.554280 | -0.368005 | -0.476089 |
| 1 | -5.859308 | 0.061237 | 1.220298 |
| 6 | -3.923199 | -2.747230 | 1.176875 |
| 1 | -4.467585 | -3.181282 | 0.327800 |
| 1 | -2.973501 | -3.290028 | 1.280009 |
| 1 | -4.518968 | -2.927965 | 2.080777 |
| 6 | 0.213861 | -1.826370 | 1.097340 |
| 8 | 0.217770 | -0.529595 | 1.008421 |
| 8 | -0.210128 | -2.602569 | 0.245049 |
| 6 | 0.819245 | -2.326341 | 2.394072 |
| 1 | 0.247080 | -1.947618 | 3.250622 |
| 1 | 0.826250 | -3.420059 | 2.411965 |
| 1 | 1.843779 | -1.947765 | 2.505000 |

**TS6**

E= -1821.1596024 a.u.

| | | | |
|---|---|---|---|
| 6 | 1.582506 | 0.289689 | -1.802941 |
| 6 | 0.714195 | 1.359542 | -1.274170 |
| 6 | 2.673024 | -0.380172 | -1.039137 |

| | | | |
|---|---|---|---|
| 6 | 3.960975 | -0.351444 | -1.583077 |
| 6 | 2.454218 | -1.069984 | 0.159227 |
| 6 | 5.015342 | -0.987290 | -0.936778 |
| 1 | 4.137411 | 0.192905 | -2.511159 |
| 6 | 3.507830 | -1.717655 | 0.792640 |
| 1 | 1.456042 | -1.115880 | 0.593313 |
| 6 | 4.790433 | -1.674176 | 0.251607 |
| 1 | 6.015090 | -0.944663 | -1.365098 |
| 1 | 3.315267 | -2.263464 | 1.715398 |
| 1 | 5.613621 | -2.178387 | 0.754862 |
| 6 | 0.973627 | 2.281986 | -0.199870 |
| 6 | 1.985351 | 2.124144 | 0.775096 |
| 6 | 0.163306 | 3.442865 | -0.141811 |
| 6 | 2.168927 | 3.081266 | 1.755446 |
| 1 | 2.631739 | 1.252770 | 0.758661 |
| 6 | 0.346387 | 4.386668 | 0.851532 |
| 1 | -0.632028 | 3.559774 | -0.874257 |
| 6 | 1.347324 | 4.208417 | 1.804480 |
| 1 | 2.954379 | 2.947056 | 2.496902 |
| 1 | -0.291408 | 5.267179 | 0.885003 |
| 1 | 1.493710 | 4.952969 | 2.585333 |
| 29 | -1.139526 | 0.442148 | -0.682734 |
| 6 | -3.296870 | 1.429150 | -1.121436 |
| 8 | -3.324706 | 0.243272 | -0.728367 |
| 8 | -2.167741 | 2.012630 | -1.313170 |
| 6 | -4.547383 | 2.210761 | -1.382649 |
| 1 | -5.431559 | 1.613228 | -1.145275 |
| 1 | -4.543898 | 3.125796 | -0.779039 |
| 1 | -4.578871 | 2.515925 | -2.435229 |
| 7 | -0.588819 | -1.427004 | -0.577414 |
| 7 | -0.152303 | -2.028774 | -1.540885 |
| 7 | 0.313495 | -2.593163 | -2.423472 |
| 1 | 0.092674 | 1.758674 | -2.082908 |
| 7 | 1.346711 | 0.021469 | -3.041818 |
| 1 | 1.975532 | -0.719143 | -3.371566 |
| 14 | -1.544004 | -2.511810 | 0.953936 |
| 6 | -2.956441 | -1.983159 | 2.097079 |
| 1 | -2.646613 | -1.842825 | 3.139456 |
| 1 | -3.351116 | -1.026344 | 1.724001 |
| 1 | -3.779703 | -2.707522 | 2.055951 |
| 6 | -2.616663 | -3.219875 | -0.466051 |
| 1 | -3.246897 | -2.436029 | -0.906850 |
| 1 | -2.049939 | -3.702726 | -1.274303 |
| 1 | -3.282240 | -3.982626 | -0.033339 |
| 6 | -0.401592 | -3.946398 | 1.381695 |
| 1 | 0.501825 | -3.890496 | 0.754103 |
| 1 | -0.073428 | -3.922161 | 2.426638 |
| 1 | -0.885037 | -4.909237 | 1.173633 |
| 6 | -0.442102 | -0.088383 | 2.180773 |
| 8 | -1.052430 | 0.734115 | 1.483627 |
| 8 | -0.379636 | -1.356241 | 1.964704 |
| 6 | 0.342939 | 0.362593 | 3.386486 |
| 1 | 1.392046 | 0.056953 | 3.271069 |
| 1 | 0.284240 | 1.448530 | 3.505222 |
| 1 | -0.037998 | -0.136385 | 4.285602 |

**I**

E= -1183.6434084 a.u.

| | | | |
|---|---|---|---|
| 6 | 0.996294 | -0.862559 | -1.027290 |
| 6 | -0.068978 | 0.160801 | -0.877177 |
| 6 | 2.408559 | -0.560849 | -0.670759 |
| 6 | 3.022212 | 0.616363 | -1.112934 |
| 6 | 3.156778 | -1.493371 | 0.054195 |
| 6 | 4.362101 | 0.854712 | -0.837164 |
| 1 | 2.449249 | 1.343908 | -1.687283 |
| 6 | 4.493045 | -1.240872 | 0.345419 |
| 1 | 2.678650 | -2.407060 | 0.410055 |
| 6 | 5.098012 | -0.070397 | -0.100999 |
| 1 | 4.833781 | 1.767235 | -1.197350 |
| 1 | 5.063150 | -1.964207 | 0.925500 |
| 1 | 6.145540 | 0.122651 | 0.124187 |
| 6 | 0.044139 | 1.438367 | -0.196417 |
| 6 | 0.833992 | 1.630334 | 0.956316 |
| 6 | -0.716187 | 2.519658 | -0.686271 |
| 6 | 0.888783 | 2.872877 | 1.562865 |
| 1 | 1.377975 | 0.789489 | 1.381171 |

| | | | |
|---|---|---|---|
| 6 | -0.647579 | 3.763234 | -0.078632 |
| 1 | -1.364207 | 2.358575 | -1.546427 |
| 6 | 0.158144 | 3.943143 | 1.043516 |
| 1 | 1.497903 | 3.011136 | 2.453630 |
| 1 | -1.229073 | 4.593458 | -0.474205 |
| 1 | 0.209439 | 4.918358 | 1.524663 |
| 29 | -1.607450 | -0.642939 | 0.197484 |
| 6 | -3.921182 | -0.361437 | -0.271593 |
| 8 | -3.651108 | -1.086637 | 0.711166 |
| 8 | -2.960341 | 0.178110 | -0.936109 |
| 6 | -5.325261 | -0.104591 | -0.716940 |
| 1 | -5.489016 | 0.972480 | -0.833921 |
| 1 | -5.483419 | -0.564761 | -1.699740 |
| 1 | -6.038911 | -0.520031 | -0.000906 |
| 7 | -0.449609 | -1.369778 | 1.496154 |
| 7 | 0.049990 | -2.440904 | 1.246847 |
| 7 | 0.575498 | -3.447135 | 1.031715 |
| 1 | -0.735196 | 0.165147 | -1.747762 |
| 7 | 0.609135 | -1.982169 | -1.524803 |
| 1 | 1.399452 | -2.625496 | -1.625313 |

**TS7**

E= -1183.6263953 a.u.

| | | | |
|---|---|---|---|
| 6 | 1.453183 | -0.634141 | -1.146294 |
| 6 | 0.307730 | 0.238260 | -0.954648 |
| 6 | 2.737480 | -0.502075 | -0.408579 |
| 6 | 3.931493 | -0.480521 | -1.135250 |
| 6 | 2.781605 | -0.458708 | 0.989582 |
| 6 | 5.153777 | -0.403749 | -0.476790 |
| 1 | 3.896078 | -0.505118 | -2.224804 |
| 6 | 4.006090 | -0.396427 | 1.642891 |
| 1 | 1.850262 | -0.489799 | 1.555162 |
| 6 | 5.191819 | -0.363786 | 0.913223 |
| 1 | 6.077383 | -0.376115 | -1.051913 |
| 1 | 4.034420 | -0.377269 | 2.730666 |
| 1 | 6.148427 | -0.308868 | 1.429844 |
| 6 | 0.237604 | 1.569691 | -0.445583 |
| 6 | 1.363338 | 2.301917 | 0.002434 |
| 6 | -1.020012 | 2.223936 | -0.502913 |
| 6 | 1.230410 | 3.625694 | 0.376414 |
| 1 | 2.342392 | 1.834309 | 0.032168 |
| 6 | -1.140429 | 3.544613 | -0.112800 |
| 1 | -1.904794 | 1.667059 | -0.818125 |
| 6 | -0.018712 | 4.246941 | 0.327054 |
| 1 | 2.103960 | 4.183315 | 0.706911 |
| 1 | -2.112597 | 4.030561 | -0.150114 |
| 1 | -0.116028 | 5.287819 | 0.631234 |
| 29 | -1.914001 | -0.819294 | 0.416777 |
| 6 | -4.367995 | -0.500593 | 0.053128 |
| 8 | -4.261217 | -1.549776 | 0.694492 |
| 8 | -3.342747 | 0.209215 | -0.299666 |
| 6 | -5.708851 | 0.043464 | -0.370260 |
| 1 | -6.516261 | -0.616244 | -0.042287 |
| 1 | -5.853665 | 1.043669 | 0.055813 |
| 1 | -5.738896 | 0.152321 | -1.460894 |
| 7 | -0.240131 | -1.521217 | 0.917228 |
| 7 | 0.217424 | -2.514531 | 0.404059 |
| 7 | 0.760737 | -3.400087 | -0.103567 |
| 1 | -0.557722 | -0.103308 | -1.527255 |
| 7 | 1.232901 | -1.576181 | -2.007700 |
| 1 | 2.057071 | -2.181307 | -2.091342 |

**J**

E= -1183.6844484 a.u.

| | | | |
|---|---|---|---|
| 6 | 1.364003 | 0.016651 | 1.341862 |
| 6 | 0.186866 | 0.376829 | 0.471979 |
| 6 | 2.303090 | -0.969476 | 0.751878 |
| 6 | 1.854247 | -2.036876 | -0.035736 |
| 6 | 3.674617 | -0.826359 | 0.987791 |
| 6 | 2.765069 | -2.952690 | -0.549523 |
| 1 | 0.791752 | -2.176572 | -0.239475 |
| 6 | 4.581787 | -1.735799 | 0.462391 |
| 1 | 4.032641 | 0.028569 | 1.562521 |
| 6 | 4.126417 | -2.805353 | -0.303776 |
| 1 | 2.405899 | -3.787006 | -1.148913 |
| 1 | 5.647257 | -1.605183 | 0.642940 |

| | | | |
|---|---|---|---|
| 1 | 4.835633 | -3.520980 | -0.716161 |
| 6 | 0.567243 | 1.190772 | -0.738807 |
| 6 | 1.518100 | 2.209654 | -0.660783 |
| 6 | -0.078794 | 0.930406 | -1.949161 |
| 6 | 1.814212 | 2.969943 | -1.786960 |
| 1 | 2.033865 | 2.401900 | 0.281600 |
| 6 | 0.222556 | 1.691765 | -3.072581 |
| 1 | -0.808391 | 0.118978 | -1.996301 |
| 6 | 1.166520 | 2.712068 | -2.991713 |
| 1 | 2.557570 | 3.762781 | -1.724362 |
| 1 | -0.277884 | 1.484811 | -4.016966 |
| 1 | 1.403773 | 3.305503 | -3.873215 |
| 29 | -2.593445 | 0.204270 | 0.815202 |
| 6 | -3.160272 | -1.791098 | -0.610025 |
| 8 | -1.923045 | -1.744062 | -0.730965 |
| 8 | -3.854342 | -0.963542 | 0.092736 |
| 6 | -3.964332 | -2.863136 | -1.302660 |
| 1 | -4.494380 | -3.464455 | -0.554612 |
| 1 | -4.729616 | -2.400926 | -1.936910 |
| 1 | -3.319877 | -3.508145 | -1.905606 |
| 7 | -0.918187 | 1.038177 | 1.247282 |
| 7 | -0.672015 | 2.142500 | 1.759404 |
| 7 | -0.520863 | 3.159743 | 2.234472 |
| 1 | -0.312651 | -0.537161 | 0.123746 |
| 7 | 1.495330 | 0.610666 | 2.462230 |
| 1 | 2.325587 | 0.273476 | 2.957898 |

**TS8**

E= -1183.6275153 a.u.

| | | | |
|---|---|---|---|
| 6 | -1.896033 | 1.271658 | -0.250832 |
| 6 | -0.524252 | 0.607743 | -0.307847 |
| 6 | -3.060319 | 0.425772 | -0.625157 |
| 6 | -2.975587 | -0.559894 | -1.613750 |
| 6 | -4.283480 | 0.617170 | 0.026901 |
| 6 | -4.091183 | -1.312624 | -1.959277 |
| 1 | -2.035968 | -0.741133 | -2.135168 |
| 6 | -5.396058 | -0.140957 | -0.309925 |
| 1 | -4.354163 | 1.349668 | 0.831694 |
| 6 | -5.303494 | -1.105405 | -1.309439 |
| 1 | -4.010219 | -2.067575 | -2.738986 |
| 1 | -6.337027 | 0.014935 | 0.214470 |
| 1 | -6.174518 | -1.701176 | -1.576188 |
| 6 | -0.412859 | -0.573384 | 0.638814 |
| 6 | -1.003486 | -0.530176 | 1.901819 |
| 6 | 0.358531 | -1.681129 | 0.279929 |
| 6 | -0.811252 | -1.574744 | 2.800660 |
| 1 | -1.611109 | 0.329242 | 2.189360 |
| 6 | 0.547562 | -2.724897 | 1.178351 |
| 1 | 0.835874 | -1.718654 | -0.702049 |
| 6 | -0.036342 | -2.672434 | 2.441180 |
| 1 | -1.269542 | -1.528519 | 3.787132 |
| 1 | 1.153488 | -3.581888 | 0.889957 |
| 1 | 0.113008 | -3.488052 | 3.146425 |
| 29 | 2.265487 | 0.701895 | -0.384804 |
| 6 | 4.215101 | -0.541436 | -0.865205 |
| 8 | 3.236721 | -0.636920 | -1.662970 |
| 8 | 4.143477 | 0.208954 | 0.153319 |
| 6 | 5.482866 | -1.295759 | -1.143839 |
| 1 | 6.014813 | -1.513818 | -0.213074 |
| 1 | 5.270529 | -2.217130 | -1.694318 |
| 1 | 6.135513 | -0.673125 | -1.768796 |
| 7 | 0.599651 | 1.488910 | -0.361191 |
| 7 | 0.496105 | 2.464078 | 1.155228 |
| 7 | 0.865867 | 3.333945 | 1.738803 |
| 1 | -0.391696 | 0.223263 | -1.345540 |
| 7 | -1.962828 | 2.472328 | 0.166340 |
| 1 | -2.929547 | 2.810883 | 0.163066 |

**K**

E= -1074.1785708 a.u.

| | | | |
|---|---|---|---|
| 6 | -1.791136 | -1.310971 | -0.531955 |
| 6 | -0.521255 | -0.782016 | 0.134861 |
| 6 | -3.087805 | -0.787057 | -0.029934 |
| 6 | -3.307627 | -0.523278 | 1.325063 |
| 6 | -4.126815 | -0.548985 | -0.936442 |
| 6 | -4.543527 | -0.066795 | 1.766276 |
| 1 | -2.514669 | -0.691193 | 2.054775 |

| | | | |
|---|---|---|---|
| 6 | -5.358213 | -0.080582 | -0.499609 |
| 1 | -3.952950 | -0.705397 | -2.001620 |
| 6 | -5.571559 | 0.155657 | 0.855483 |
| 1 | -4.703397 | 0.119457 | 2.826662 |
| 1 | -6.151441 | 0.108884 | -1.220514 |
| 1 | -6.536098 | 0.522932 | 1.201335 |
| 6 | -0.343437 | 0.715684 | -0.060221 |
| 6 | -0.683814 | 1.317717 | -1.270927 |
| 6 | 0.242270 | 1.484927 | 0.946988 |
| 6 | -0.433301 | 2.671323 | -1.473265 |
| 1 | -1.134044 | 0.720311 | -2.064199 |
| 6 | 0.489916 | 2.837716 | 0.745399 |
| 1 | 0.516978 | 1.016099 | 1.894591 |
| 6 | 0.151564 | 3.433218 | -0.466728 |
| 1 | -0.693238 | 3.131922 | -2.424849 |
| 1 | 0.946188 | 3.428048 | 1.538078 |
| 1 | 0.344865 | 4.492514 | -0.626746 |
| 29 | 2.260391 | -0.988055 | 0.057317 |
| 6 | 4.457389 | -0.228298 | 0.173026 |
| 8 | 3.801835 | -0.443148 | 1.236878 |
| 8 | 3.900618 | -0.445652 | -0.946134 |
| 6 | 5.856637 | 0.295014 | 0.226838 |
| 1 | 6.475467 | -0.213558 | -0.519428 |
| 1 | 5.850026 | 1.362420 | -0.025981 |
| 1 | 6.280041 | 0.170339 | 1.227070 |
| 7 | 0.595542 | -1.604319 | 0.012101 |
| 1 | -0.628036 | -0.968227 | 1.241859 |
| 7 | -1.637876 | -2.089404 | -1.528827 |
| 1 | -2.550048 | -2.374147 | -1.901214 |

**TS9**

E= -1419.5081252 a.u.

| | | | |
|---|---|---|---|
| 6 | -0.183337 | 1.772451 | -1.214100 |
| 6 | -0.702728 | 0.644434 | -0.172702 |
| 6 | 1.219679 | 2.216061 | -1.110711 |
| 6 | 1.475858 | 3.591534 | -1.063807 |
| 6 | 2.284159 | 1.312936 | -1.091286 |
| 6 | 2.782776 | 4.056168 | -1.002728 |
| 1 | 0.641948 | 4.293832 | -1.050362 |
| 6 | 3.589959 | 1.783877 | -1.037686 |
| 1 | 2.106219 | 0.239729 | -1.118196 |
| 6 | 3.842179 | 3.151813 | -0.991610 |
| 1 | 2.974996 | 5.126650 | -0.956297 |
| 1 | 4.407704 | 1.066050 | -1.021984 |
| 1 | 4.866704 | 3.516559 | -0.938610 |
| 6 | -0.210538 | 0.859710 | 1.238646 |
| 6 | 0.972202 | 0.323567 | 1.752553 |
| 6 | -1.022545 | 1.636518 | 2.067491 |
| 6 | 1.322839 | 0.561732 | 3.077409 |
| 1 | 1.638018 | -0.275284 | 1.127975 |
| 6 | -0.666609 | 1.879716 | 3.389174 |
| 1 | -1.952562 | 2.045902 | 1.666864 |
| 6 | 0.510253 | 1.339597 | 3.897510 |
| 1 | 2.245010 | 0.135672 | 3.469212 |
| 1 | -1.311247 | 2.486697 | 4.023087 |
| 1 | 0.792399 | 1.521245 | 4.933384 |
| 29 | 0.499145 | -1.969810 | -0.357872 |
| 6 | 2.804108 | -2.858212 | -0.000497 |
| 8 | 2.907880 | -1.628660 | -0.202606 |
| 8 | 1.670573 | -3.449934 | 0.016802 |
| 6 | 4.025193 | -3.712189 | 0.207012 |
| 1 | 4.896606 | -3.097939 | 0.450556 |
| 1 | 3.843662 | -4.450135 | 0.995443 |
| 1 | 4.232886 | -4.268361 | -0.715837 |
| 7 | -0.338739 | -0.420214 | -0.971279 |
| 1 | -1.786408 | 0.873123 | -0.206411 |
| 7 | -1.087909 | 2.224910 | -1.974179 |
| 1 | -0.711528 | 2.969293 | -2.571261 |
| 6 | -2.068698 | -1.823393 | -1.148935 |
| 1 | -1.918927 | -1.904680 | -2.239376 |
| 6 | -3.195957 | -1.009646 | -0.710043 |
| 6 | -3.839569 | -0.183548 | -1.635446 |
| 6 | -3.567824 | -0.979276 | 0.639016 |
| 6 | -4.857529 | 0.663028 | -1.217861 |
| 1 | -3.510945 | -0.188859 | -2.674929 |
| 6 | -4.593489 | -0.140182 | 1.050347 |

| | | | |
|---|---|---|---|
| 1 | -3.035858 | -1.615685 | 1.344657 |
| 6 | -5.236624 | 0.679292 | 0.122664 |
| 1 | -5.351763 | 1.316280 | -1.933908 |
| 1 | -4.890417 | -0.116619 | 2.097212 |
| 1 | -6.036627 | 1.341789 | 0.449561 |
| 8 | -1.419840 | -2.561352 | -0.364291 |

**L**

E= -1419.5502585 a.u.

| | | | |
|---|---|---|---|
| 6 | -1.409920 | 0.573884 | -1.134401 |
| 6 | -0.221534 | 0.113276 | -0.292660 |
| 6 | -2.402202 | 1.410985 | -0.413093 |
| 6 | -2.985092 | 0.989546 | 0.785618 |
| 6 | -2.773512 | 2.642114 | -0.961471 |
| 6 | -3.941280 | 1.782099 | 1.410208 |
| 1 | -2.715921 | 0.022491 | 1.213815 |
| 6 | -3.717063 | 3.439146 | -0.325967 |
| 1 | -2.291678 | 2.980884 | -1.879349 |
| 6 | -4.305258 | 3.007459 | 0.859564 |
| 1 | -4.404903 | 1.439776 | 2.333817 |
| 1 | -3.989319 | 4.402738 | -0.753038 |
| 1 | -5.046731 | 3.629674 | 1.357813 |
| 6 | 0.649174 | 1.310437 | 0.019825 |
| 6 | 1.119247 | 2.129959 | -1.006007 |
| 6 | 0.999575 | 1.587541 | 1.339985 |
| 6 | 1.935413 | 3.213753 | -0.711385 |
| 1 | 0.853997 | 1.894547 | -2.037169 |
| 6 | 1.824254 | 2.669532 | 1.634608 |
| 1 | 0.623042 | 0.948712 | 2.141511 |
| 6 | 2.289447 | 3.485071 | 0.608238 |
| 1 | 2.304304 | 3.847912 | -1.515754 |
| 1 | 2.093307 | 2.880860 | 2.668331 |
| 1 | 2.927982 | 4.336938 | 0.837460 |
| 29 | 2.161199 | -1.211269 | -0.135267 |
| 6 | 4.316859 | -0.392517 | 0.180415 |
| 8 | 3.494483 | 0.169060 | -0.610917 |
| 8 | 3.941347 | -1.440901 | 0.782482 |
| 6 | 5.679304 | 0.183387 | 0.374879 |
| 1 | 6.214254 | -0.342094 | 1.170243 |
| 1 | 6.244190 | 0.103991 | -0.561465 |
| 1 | 5.592428 | 1.249495 | 0.612546 |
| 7 | 0.505381 | -0.925230 | -1.016159 |
| 1 | -0.623097 | -0.273201 | 0.661335 |
| 7 | -1.446152 | 0.301201 | -2.378904 |
| 1 | -2.291566 | 0.710240 | -2.791738 |
| 6 | 0.028888 | -2.300862 | -0.705719 |
| 1 | 0.162478 | -2.891233 | -1.628972 |
| 6 | -1.367269 | -2.493472 | -0.185912 |
| 6 | -2.440118 | -2.536140 | -1.079003 |
| 6 | -1.605492 | -2.644090 | 1.180835 |
| 6 | -3.737862 | -2.694124 | -0.609318 |
| 1 | -2.246886 | -2.422354 | -2.146080 |
| 6 | -2.905087 | -2.818377 | 1.650114 |
| 1 | -0.757076 | -2.638128 | 1.863052 |
| 6 | -3.972557 | -2.834812 | 0.757310 |
| 1 | -4.570390 | -2.716509 | -1.310525 |
| 1 | -3.083279 | -2.945614 | 2.716951 |
| 1 | -4.988998 | -2.967666 | 1.124645 |
| 8 | 1.008796 | -2.565562 | 0.247283 |

**M**

E= -1648.5129531 a.u.

| | | | |
|---|---|---|---|
| 6 | -1.734465 | 0.393037 | -0.919431 |
| 6 | -0.730114 | 0.276013 | 0.214815 |
| 6 | -2.835754 | 1.359318 | -0.680098 |
| 6 | -3.646926 | 1.255696 | 0.453642 |
| 6 | -3.092521 | 2.361290 | -1.619793 |
| 6 | -4.704508 | 2.139104 | 0.636214 |
| 1 | -3.472800 | 0.458447 | 1.179099 |
| 6 | -4.139365 | 3.253564 | -1.425374 |
| 1 | -2.444896 | 2.450506 | -2.492738 |
| 6 | -4.947931 | 3.141977 | -0.297800 |
| 1 | -5.342035 | 2.045287 | 1.513462 |
| 1 | -4.321163 | 4.041597 | -2.153942 |
| 1 | -5.768450 | 3.840877 | -0.145530 |
| 6 | 0.181830 | 1.485898 | 0.256280 |

| | | | |
|---|---|---|---|
| 6 | 0.691080 | 2.042375 | -0.918468 |
| 6 | 0.591484 | 1.990168 | 1.492137 |
| 6 | 1.609611 | 3.084480 | -0.852192 |
| 1 | 0.398234 | 1.627291 | -1.881901 |
| 6 | 1.509888 | 3.029978 | 1.556345 |
| 1 | 0.220588 | 1.528239 | 2.406736 |
| 6 | 2.019302 | 3.578046 | 0.382827 |
| 1 | 2.013532 | 3.504758 | -1.771462 |
| 1 | 1.843882 | 3.399333 | 2.523614 |
| 1 | 2.745795 | 4.387422 | 0.432375 |
| 29 | 1.980774 | -0.708977 | 0.127767 |
| 6 | 1.976301 | -1.836696 | -2.168283 |
| 8 | 2.015455 | -0.605130 | -1.762521 |
| 8 | 1.936872 | -2.799672 | -1.399633 |
| 6 | 1.955084 | -1.986286 | -3.667115 |
| 1 | 2.065479 | -3.039294 | -3.940491 |
| 1 | 0.998985 | -1.604669 | -4.045827 |
| 1 | 2.752518 | -1.390402 | -4.123785 |
| 7 | 0.064577 | -0.956152 | 0.106038 |
| 1 | -1.280385 | 0.241723 | 1.166198 |
| 7 | -1.562510 | -0.268723 | -1.994553 |
| 1 | -2.315806 | -0.050623 | -2.654698 |
| 6 | -0.436695 | -2.118389 | 0.244910 |
| 6 | -1.839264 | -2.361156 | 0.643776 |
| 6 | -2.790781 | -2.840792 | -0.255604 |
| 6 | -2.192490 | -2.104129 | 1.971874 |
| 6 | -4.098936 | -3.042948 | 0.170321 |
| 1 | -2.504861 | -3.029288 | -1.289223 |
| 6 | -3.500077 | -2.321534 | 2.393913 |
| 1 | -1.429900 | -1.744610 | 2.665487 |
| 6 | -4.454400 | -2.783402 | 1.491340 |
| 1 | -4.844499 | -3.408431 | -0.533356 |
| 1 | -3.772363 | -2.130304 | 3.430374 |
| 1 | -5.478837 | -2.947984 | 1.820516 |
| 8 | 1.797878 | -0.926773 | 1.901701 |
| 1 | 2.517642 | -0.372529 | 2.279143 |
| 1 | 0.253445 | -2.955215 | 0.097469 |
| 6 | 4.405912 | 0.340220 | 1.074561 |
| 8 | 3.947354 | 0.714714 | 2.146474 |
| 8 | 3.781348 | -0.318349 | 0.138348 |
| 6 | 5.839537 | 0.617515 | 0.676832 |
| 1 | 6.348813 | -0.322379 | 0.437393 |
| 1 | 5.858180 | 1.237134 | -0.226804 |
| 1 | 6.355918 | 1.129177 | 1.493528 |

**TS10**

E= -1648.4884142 a.u.

| | | | |
|---|---|---|---|
| 6 | -1.642131 | 0.476632 | -1.011852 |
| 6 | -1.141276 | -0.364641 | 0.154777 |
| 6 | -2.558601 | 1.613264 | -0.741770 |
| 6 | -3.578021 | 1.525975 | 0.212043 |
| 6 | -2.440286 | 2.780173 | -1.502151 |
| 6 | -4.470738 | 2.576446 | 0.383873 |
| 1 | -3.679188 | 0.628993 | 0.822117 |
| 6 | -3.322517 | 3.837351 | -1.316631 |
| 1 | -1.630704 | 2.864206 | -2.226858 |
| 6 | -4.343071 | 3.735460 | -0.376421 |
| 1 | -5.267596 | 2.490394 | 1.120349 |
| 1 | -3.209541 | 4.745987 | -1.905236 |
| 1 | -5.037901 | 4.560901 | -0.232390 |
| 6 | -1.042886 | 0.241240 | 1.537019 |
| 6 | -0.631917 | 1.553772 | 1.781156 |
| 6 | -1.322464 | -0.597535 | 2.619116 |
| 6 | -0.517791 | 2.013684 | 3.088977 |
| 1 | -0.391012 | 2.207835 | 0.946743 |
| 6 | -1.208653 | -0.136545 | 3.924788 |
| 1 | -1.622936 | -1.630504 | 2.429121 |
| 6 | -0.807233 | 1.174988 | 4.160644 |
| 1 | -0.196720 | 3.038030 | 3.268930 |
| 1 | -1.432042 | -0.801056 | 4.757498 |
| 1 | -0.715701 | 1.542890 | 5.181205 |
| 29 | 1.825431 | 0.072688 | 0.098562 |
| 6 | 1.510926 | 1.526692 | -1.915091 |
| 8 | 1.009771 | 1.579982 | -0.711540 |
| 8 | 2.249855 | 0.624822 | -2.295954 |
| 6 | 1.092276 | 2.652244 | -2.828222 |

| | | | |
|---|---|---|---|
| 1 | 0.320653 | 2.274148 | -3.512605 |
| 1 | 0.698910 | 3.510008 | -2.273632 |
| 1 | 1.947020 | 2.957706 | -3.440287 |
| 7 | 0.151276 | -1.015630 | -0.147251 |
| 1 | -1.862115 | -1.201975 | 0.223879 |
| 7 | -1.343660 | 0.064811 | -2.182077 |
| 1 | -1.809782 | 0.643021 | -2.887566 |
| 6 | 0.383487 | -2.246300 | -0.259580 |
| 6 | -0.553963 | -3.345877 | -0.443250 |
| 6 | -1.621668 | -3.240375 | -1.346935 |
| 6 | -0.355355 | -4.534070 | 0.270426 |
| 6 | -2.492325 | -4.311539 | -1.506318 |
| 1 | -1.726242 | -2.329312 | -1.938787 |
| 6 | -1.250413 | -5.584979 | 0.127522 |
| 1 | 0.498328 | -4.614921 | 0.942269 |
| 6 | -2.316318 | -5.476137 | -0.763246 |
| 1 | -3.313145 | -4.236946 | -2.217453 |
| 1 | -1.106466 | -6.500783 | 0.697687 |
| 1 | -3.006041 | -6.309046 | -0.888349 |
| 8 | 2.541141 | -1.559116 | 0.584492 |
| 1 | 3.485519 | -1.531280 | 0.262300 |
| 1 | 1.695989 | -2.280954 | 0.033655 |
| 6 | 4.548042 | 0.619867 | 0.239830 |
| 8 | 4.848513 | -0.526705 | -0.087985 |
| 8 | 3.361286 | 1.067309 | 0.511929 |
| 6 | 5.604123 | 1.696757 | 0.363403 |
| 1 | 5.446586 | 2.445278 | -0.421711 |
| 1 | 5.512097 | 2.208795 | 1.327098 |
| 1 | 6.599324 | 1.256747 | 0.258837 |

**N**

E= -1572.1656863 a.u.

| | | | |
|---|---|---|---|
| 6 | -1.742116 | -1.380715 | 0.903393 |
| 6 | -1.084027 | -0.201782 | 1.616561 |
| 6 | -3.188908 | -1.238233 | 0.613266 |
| 6 | -4.086963 | -0.744947 | 1.563902 |
| 6 | -3.658395 | -1.624042 | -0.647336 |
| 6 | -5.443017 | -0.672534 | 1.271300 |
| 1 | -3.733228 | -0.428735 | 2.545582 |
| 6 | -5.013716 | -1.534322 | -0.938855 |
| 1 | -2.936828 | -1.929653 | -1.407344 |
| 6 | -5.908293 | -1.068560 | 0.020403 |
| 1 | -6.139573 | -0.301122 | 2.020912 |
| 1 | -5.371648 | -1.820285 | -1.926307 |
| 1 | -6.970245 | -1.002898 | -0.210424 |
| 6 | -1.346673 | 1.155800 | 1.003400 |
| 6 | -1.421623 | 1.322656 | -0.380459 |
| 6 | -1.447642 | 2.260771 | 1.847098 |
| 6 | -1.593927 | 2.599631 | -0.908207 |
| 1 | -1.350720 | 0.462162 | -1.052697 |
| 6 | -1.622643 | 3.532421 | 1.315777 |
| 1 | -1.382178 | 2.122917 | 2.927613 |
| 6 | -1.695409 | 3.701703 | -0.064971 |
| 1 | -1.634479 | 2.726679 | -1.987905 |
| 1 | -1.704324 | 4.391716 | 1.979367 |
| 1 | -1.832600 | 4.697203 | -0.485317 |
| 29 | 1.317060 | 0.397596 | -0.853899 |
| 6 | 0.248939 | -1.865515 | -2.013334 |
| 8 | -0.814035 | -1.267437 | -2.182202 |
| 8 | 1.319006 | -1.374448 | -1.478901 |
| 6 | 0.405069 | -3.315028 | -2.420087 |
| 1 | 1.214029 | -3.416969 | -3.152940 |
| 1 | 0.689600 | -3.908395 | -1.541046 |
| 1 | -0.526030 | -3.701566 | -2.845971 |
| 7 | 0.336296 | -0.452934 | 1.718727 |
| 1 | -1.460401 | -0.188930 | 2.652629 |
| 7 | -1.026979 | -2.388650 | 0.604273 |
| 1 | -1.605697 | -3.094383 | 0.138373 |
| 6 | 1.355340 | -0.489704 | 1.097071 |
| 6 | 2.724441 | -0.937657 | 1.111081 |
| 6 | 2.947607 | -2.315439 | 0.992174 |
| 6 | 3.782137 | -0.028424 | 1.226355 |
| 6 | 4.251437 | -2.784888 | 1.030045 |
| 1 | 2.094612 | -2.979061 | 0.863068 |
| 6 | 5.078158 | -0.520666 | 1.269022 |
| 1 | 3.564883 | 1.037410 | 1.259065 |

| | | | |
|---|---|---|---|
| 6 | 5.311878 | -1.891399 | 1.172026 |
| 1 | 4.443586 | -3.852109 | 0.941809 |
| 1 | 5.912773 | 0.169957 | 1.369004 |
| 1 | 6.333161 | -2.267255 | 1.198479 |
| 6 | 1.711052 | 2.789681 | -0.999069 |
| 8 | 1.764255 | 2.063969 | 0.065494 |
| 8 | 1.451182 | 2.292760 | -2.108725 |
| 6 | 1.967087 | 4.260164 | -0.824067 |
| 1 | 1.890219 | 4.782611 | -1.781382 |
| 1 | 1.239917 | 4.670925 | -0.113187 |
| 1 | 2.963208 | 4.418006 | -0.393573 |

**O**

E= -1572.1729882 a.u.

| | | | |
|---|---|---|---|
| 6 | 1.603303 | -0.404830 | 0.173893 |
| 6 | 1.162635 | 0.418814 | -1.033863 |
| 6 | 3.018670 | -0.840492 | 0.126714 |
| 6 | 3.454740 | -1.737292 | -0.852905 |
| 6 | 3.918011 | -0.340660 | 1.071267 |
| 6 | 4.786839 | -2.135075 | -0.871192 |
| 1 | 2.728105 | -2.153678 | -1.550808 |
| 6 | 5.251008 | -0.732066 | 1.035773 |
| 1 | 3.568146 | 0.377754 | 1.813669 |
| 6 | 5.685409 | -1.630103 | 0.064971 |
| 1 | 5.125789 | -2.848504 | -1.620479 |
| 1 | 5.953167 | -0.331911 | 1.765072 |
| 1 | 6.729131 | -1.938918 | 0.039134 |
| 6 | 1.696710 | 1.825434 | -0.815579 |
| 6 | 1.048238 | 2.673472 | 0.085113 |
| 6 | 2.853387 | 2.249406 | -1.463073 |
| 6 | 1.552944 | 3.947966 | 0.314917 |
| 1 | 0.152486 | 2.331422 | 0.609234 |
| 6 | 3.359220 | 3.523567 | -1.224179 |
| 1 | 3.361788 | 1.574779 | -2.153084 |
| 6 | 2.706985 | 4.374676 | -0.338297 |
| 1 | 1.043747 | 4.610955 | 1.012256 |
| 1 | 4.262856 | 3.851468 | -1.734984 |
| 1 | 3.099780 | 5.373332 | -0.154352 |
| 29 | -1.311055 | -0.814360 | 0.896280 |
| 6 | -1.984958 | 0.288139 | 2.929093 |
| 8 | -1.683302 | -0.925517 | 3.025579 |
| 8 | -1.980406 | 0.881503 | 1.796891 |
| 6 | -2.373727 | 1.068780 | 4.154135 |
| 1 | -1.628786 | 0.912952 | 4.942465 |
| 1 | -2.473383 | 2.135527 | 3.935024 |
| 1 | -3.329093 | 0.687732 | 4.534872 |
| 7 | -0.240074 | 0.482268 | -1.279514 |
| 1 | 1.620377 | -0.017302 | -1.931914 |
| 7 | 0.835532 | -0.534502 | 1.177471 |
| 1 | 1.267624 | -1.050941 | 1.946206 |
| 6 | -1.316212 | 0.134189 | -0.854983 |
| 6 | -2.706581 | 0.415347 | -1.180674 |
| 6 | -3.699634 | -0.567441 | -1.148954 |
| 6 | -3.015356 | 1.741375 | -1.512139 |
| 6 | -5.001265 | -0.219392 | -1.484548 |
| 1 | -3.429675 | -1.584426 | -0.869475 |
| 6 | -4.321897 | 2.074268 | -1.834790 |
| 1 | -2.222740 | 2.488220 | -1.510487 |
| 6 | -5.313012 | 1.094756 | -1.823597 |
| 1 | -5.779605 | -0.979594 | -1.474161 |
| 1 | -4.569599 | 3.101733 | -2.094085 |
| 1 | -6.338140 | 1.359823 | -2.076817 |
| 6 | -0.585217 | -2.950337 | -0.891230 |
| 8 | -1.502441 | -2.441710 | -0.129432 |
| 8 | 0.421402 | -2.378611 | -1.311514 |
| 6 | -0.863635 | -4.395296 | -1.253464 |
| 1 | -0.112155 | -4.768199 | -1.955172 |
| 1 | -0.855262 | -5.008943 | -0.344586 |
| 1 | -1.863845 | -4.489742 | -1.691982 |

**TS11**

E= -1572.1573533 a.u.

| | | | |
|---|---|---|---|
| 6 | 1.315436 | -0.605831 | 0.641105 |
| 6 | 1.255413 | 0.666214 | -0.093310 |
| 6 | 2.619141 | -1.297078 | 0.754585 |
| 6 | 3.461706 | -1.417243 | -0.355158 |

| | | | |
|---|---|---|---|
| 6 | 2.995933 | -1.863925 | 1.975244 |
| 6 | 4.665756 | -2.099046 | -0.237156 |
| 1 | 3.158114 | -0.998552 | -1.314084 |
| 6 | 4.210190 | -2.529842 | 2.090823 |
| 1 | 2.342153 | -1.757875 | 2.841297 |
| 6 | 5.045872 | -2.648158 | 0.984723 |
| 1 | 5.312959 | -2.200168 | -1.106154 |
| 1 | 4.504881 | -2.955701 | 3.048175 |
| 1 | 5.996351 | -3.171266 | 1.074435 |
| 6 | 2.459286 | 1.565823 | -0.124201 |
| 6 | 3.142586 | 1.916690 | 1.041667 |
| 6 | 2.878457 | 2.096135 | -1.344827 |
| 6 | 4.230143 | 2.780008 | 0.988357 |
| 1 | 2.817896 | 1.503769 | 1.998162 |
| 6 | 3.964251 | 2.963809 | -1.399210 |
| 1 | 2.346102 | 1.813505 | -2.253667 |
| 6 | 4.642580 | 3.305315 | -0.233582 |
| 1 | 4.758492 | 3.044683 | 1.903011 |
| 1 | 4.285663 | 3.370174 | -2.356911 |
| 1 | 5.495705 | 3.980692 | -0.275543 |
| 29 | -1.538940 | -0.911893 | 0.263651 |
| 6 | -3.425570 | -2.383849 | 0.369043 |
| 8 | -3.544887 | -1.114732 | 0.353893 |
| 8 | -2.289619 | -2.923326 | 0.378141 |
| 6 | -4.673679 | -3.219912 | 0.352159 |
| 1 | -4.444159 | -4.266997 | 0.568927 |
| 1 | -5.399210 | -2.831121 | 1.075054 |
| 1 | -5.136437 | -3.153277 | -0.640257 |
| 7 | 0.052979 | 1.376358 | 0.122887 |
| 1 | 1.041290 | 0.208476 | -1.289646 |
| 7 | 0.227142 | -1.154038 | 1.073163 |
| 1 | 0.348858 | -2.108338 | 1.413318 |
| 6 | -1.118796 | 1.120195 | 0.270525 |
| 6 | -2.408168 | 1.723982 | 0.501394 |
| 6 | -3.388572 | 1.661439 | -0.496857 |
| 6 | -2.656502 | 2.373018 | 1.718328 |
| 6 | -4.603297 | 2.295258 | -0.285959 |
| 1 | -3.177002 | 1.105812 | -1.408448 |
| 6 | -3.880401 | 2.992801 | 1.916793 |
| 1 | -1.882237 | 2.396653 | 2.482747 |
| 6 | -4.849236 | 2.956531 | 0.915182 |
| 1 | -5.369789 | 2.259903 | -1.056961 |
| 1 | -4.080549 | 3.508779 | 2.853665 |
| 1 | -5.809837 | 3.442961 | 1.076406 |
| 6 | -0.406822 | -0.591337 | -2.736998 |
| 8 | -1.340110 | -0.594778 | -1.908111 |
| 8 | 0.801546 | -0.235584 | -2.519547 |
| 6 | -0.684099 | -1.059356 | -4.146209 |
| 1 | -0.215484 | -2.040669 | -4.291682 |
| 1 | -1.758872 | -1.151199 | -4.322944 |
| 1 | -0.231582 | -0.374080 | -4.870920 |

**P**

E= -1343.2166117 a.u.

| | | | |
|---|---|---|---|
| 6 | -1.093839 | -0.464373 | 0.588756 |
| 6 | -1.085206 | 0.769541 | -0.138362 |
| 6 | -2.360729 | -1.124231 | 0.983056 |
| 6 | -3.356583 | -0.406770 | 1.651539 |
| 6 | -2.550012 | -2.485736 | 0.726101 |
| 6 | -4.523981 | -1.042229 | 2.053507 |
| 1 | -3.206927 | 0.652455 | 1.857246 |
| 6 | -3.726003 | -3.114853 | 1.118063 |
| 1 | -1.778644 | -3.043801 | 0.193472 |
| 6 | -4.713975 | -2.395180 | 1.783262 |
| 1 | -5.291616 | -0.478327 | 2.580415 |
| 1 | -3.871184 | -4.171619 | 0.900829 |
| 1 | -5.633175 | -2.889400 | 2.092895 |
| 6 | -2.231881 | 1.421539 | -0.795159 |
| 6 | -3.277933 | 0.697169 | -1.381849 |
| 6 | -2.253275 | 2.818827 | -0.895393 |
| 6 | -4.317766 | 1.352879 | -2.028317 |
| 1 | -3.270502 | -0.390929 | -1.347227 |
| 6 | -3.290147 | 3.471756 | -1.548673 |
| 1 | -1.440837 | 3.390690 | -0.447833 |
| 6 | -4.331420 | 2.741926 | -2.113897 |
| 1 | -5.117562 | 0.770115 | -2.482576 |

| | | | |
|---|---|---|---|
| 1 | -3.286679 | 4.558809 | -1.612137 |
| 1 | -5.146831 | 3.252482 | -2.623505 |
| 29 | 1.590557 | -1.090307 | -0.251544 |
| 6 | 3.040188 | -2.782516 | -1.111955 |
| 8 | 1.985904 | -3.178909 | -0.553177 |
| 8 | 3.299215 | -1.536046 | -1.204334 |
| 6 | 4.024348 | -3.757646 | -1.690008 |
| 1 | 5.007419 | -3.606625 | -1.228899 |
| 1 | 3.694317 | -4.787524 | -1.531450 |
| 1 | 4.142009 | -3.566801 | -2.763121 |
| 7 | 0.116532 | 1.307345 | -0.311988 |
| 7 | 0.057667 | -1.013779 | 0.926616 |
| 1 | -0.072650 | -1.920678 | 1.375935 |
| 6 | 1.308958 | 0.954681 | -0.225109 |
| 6 | 2.416534 | 1.685066 | 0.378298 |
| 6 | 2.155208 | 2.810772 | 1.178156 |
| 6 | 3.740408 | 1.278440 | 0.162772 |
| 6 | 3.201235 | 3.517226 | 1.748101 |
| 1 | 1.121915 | 3.117079 | 1.336520 |
| 6 | 4.783011 | 1.991813 | 0.741168 |
| 1 | 3.938017 | 0.403013 | -0.454839 |
| 6 | 4.516641 | 3.106453 | 1.530585 |
| 1 | 2.995220 | 4.389630 | 2.365717 |
| 1 | 5.810645 | 1.676571 | 0.571270 |
| 1 | 5.337875 | 3.661135 | 1.981921 |

**TS12**

E= -1343.2086371 a.u.

| | | | |
|---|---|---|---|
| 6 | -0.971714 | 0.197148 | 0.654944 |
| 6 | -1.106168 | -0.927659 | -0.186494 |
| 6 | -2.060933 | 1.102157 | 1.072040 |
| 6 | -2.920303 | 1.674889 | 0.128269 |
| 6 | -2.213682 | 1.431492 | 2.422929 |
| 6 | -3.910223 | 2.560935 | 0.532038 |
| 1 | -2.802715 | 1.425055 | -0.925273 |
| 6 | -3.211779 | 2.311808 | 2.824733 |
| 1 | -1.555180 | 0.974554 | 3.162236 |
| 6 | -4.060626 | 2.878808 | 1.879753 |
| 1 | -4.568971 | 3.007423 | -0.210554 |
| 1 | -3.327323 | 2.553353 | 3.879848 |
| 1 | -4.840792 | 3.570296 | 2.193091 |
| 6 | -2.336145 | -1.494958 | -0.757012 |
| 6 | -3.554841 | -1.473876 | -0.067357 |
| 6 | -2.285315 | -2.116551 | -2.010528 |
| 6 | -4.693388 | -2.037694 | -0.629160 |
| 1 | -3.609247 | -1.025290 | 0.923427 |
| 6 | -3.423888 | -2.683839 | -2.567649 |
| 1 | -1.335602 | -2.150096 | -2.542788 |
| 6 | -4.634451 | -2.641370 | -1.881850 |
| 1 | -5.631694 | -2.015094 | -0.077112 |
| 1 | -3.365211 | -3.159126 | -3.545598 |
| 1 | -5.528283 | -3.083477 | -2.319040 |
| 29 | 1.521148 | 0.963226 | -0.447987 |
| 6 | 2.786503 | 2.707052 | -1.438358 |
| 8 | 3.029338 | 1.497513 | -1.738676 |
| 8 | 1.871328 | 2.994711 | -0.614369 |
| 6 | 3.570977 | 3.807297 | -2.092710 |
| 1 | 3.715651 | 4.637982 | -1.395064 |
| 1 | 4.532798 | 3.437762 | -2.459386 |
| 1 | 3.000018 | 4.188684 | -2.948624 |
| 7 | 0.076788 | -1.502410 | -0.458497 |
| 7 | 0.291687 | 0.442703 | 1.038787 |
| 1 | 0.397791 | 1.277332 | 1.620318 |
| 6 | 1.187382 | -0.991796 | -0.109558 |
| 6 | 2.335206 | -1.656499 | 0.501896 |
| 6 | 3.620437 | -1.109109 | 0.409239 |
| 6 | 2.142575 | -2.868233 | 1.180951 |
| 6 | 4.693940 | -1.759088 | 1.005393 |
| 1 | 3.776125 | -0.187560 | -0.154469 |
| 6 | 3.219519 | -3.514558 | 1.767966 |
| 1 | 1.139157 | -3.287284 | 1.234651 |
| 6 | 4.494715 | -2.957116 | 1.685018 |
| 1 | 5.692413 | -1.333243 | 0.928092 |
| 1 | 3.067542 | -4.455552 | 2.293699 |
| 1 | 5.338800 | -3.464569 | 2.149541 |

**3b**

E= -918.6755575 a.u.

| | | | |
|---|---|---|---|
| 6 | 0.443296 | -0.682538 | -0.015694 |
| 6 | 0.365163 | 0.703634 | -0.039377 |
| 6 | -1.674612 | 0.005825 | -0.013889 |
| 6 | 1.529202 | -1.656395 | 0.053686 |
| 6 | 1.412024 | -2.891247 | -0.598625 |
| 6 | 2.684765 | -1.404059 | 0.805795 |
| 6 | 2.416422 | -3.846811 | -0.500157 |
| 1 | 0.534635 | -3.091939 | -1.214670 |
| 6 | 3.690787 | -2.356198 | 0.893147 |
| 1 | 2.781509 | -0.453687 | 1.328684 |
| 6 | 3.560789 | -3.582462 | 0.244777 |
| 1 | 2.307380 | -4.799355 | -1.016389 |
| 1 | 4.580121 | -2.142942 | 1.484003 |
| 1 | 4.349195 | -4.329071 | 0.321884 |
| 6 | 1.433454 | 1.706995 | -0.096491 |
| 6 | 1.215690 | 2.964241 | 0.478386 |
| 6 | 2.653865 | 1.463426 | -0.737060 |
| 6 | 2.200997 | 3.941713 | 0.437170 |
| 1 | 0.255706 | 3.157472 | 0.953801 |
| 6 | 3.638861 | 2.442520 | -0.776656 |
| 1 | 2.823610 | 0.503142 | -1.222794 |
| 6 | 3.419169 | 3.683673 | -0.185677 |
| 1 | 2.017680 | 4.913117 | 0.894476 |
| 1 | 4.581039 | 2.238006 | -1.283345 |
| 1 | 4.191731 | 4.450315 | -0.219067 |
| 7 | -0.946314 | 1.102476 | -0.029837 |
| 6 | -3.132534 | -0.037162 | -0.000963 |
| 6 | -3.848475 | -1.238578 | -0.025950 |
| 6 | -3.839433 | 1.170655 | 0.035964 |
| 6 | -5.237512 | -1.233309 | -0.009462 |
| 1 | -3.327927 | -2.196093 | -0.067239 |
| 6 | -5.225988 | 1.172386 | 0.050022 |
| 1 | -3.271906 | 2.098803 | 0.050314 |
| 6 | -5.932169 | -0.028512 | 0.028973 |
| 1 | -5.779820 | -2.177188 | -0.029515 |
| 1 | -5.762523 | 2.119461 | 0.077352 |
| 1 | -7.020573 | -0.025037 | 0.040651 |
| 7 | -0.873493 | -1.101011 | -0.022176 |
| 1 | -1.163776 | -2.062019 | 0.098436 |

**TS13**

E= -1268.9987041 a.u.

| | | | |
|---|---|---|---|
| 6 | 0.268618 | 0.204651 | -1.889009 |
| 8 | 1.263756 | -0.310838 | -2.601465 |
| 6 | 0.458881 | 1.505870 | -1.370292 |
| 1 | 0.947427 | 2.158263 | -2.109984 |
| 6 | -0.514472 | 2.203809 | -0.491051 |
| 6 | -0.703317 | 1.797140 | 0.831668 |
| 6 | -1.270112 | 3.272563 | -0.982736 |
| 6 | -1.670415 | 2.401693 | 1.626304 |
| 1 | -0.103889 | 0.993877 | 1.262644 |
| 6 | -2.227447 | 3.889200 | -0.183777 |
| 1 | -1.118803 | 3.608014 | -2.010008 |
| 6 | -2.440039 | 3.445032 | 1.119168 |
| 1 | -1.807076 | 2.045540 | 2.646163 |
| 1 | -2.813447 | 4.715969 | -0.582594 |
| 1 | -3.196546 | 3.921187 | 1.740952 |
| 29 | 1.333525 | -1.095860 | 0.949847 |
| 8 | 3.091153 | -0.473942 | 0.717238 |
| 8 | -0.321642 | -0.509439 | 2.950016 |
| 6 | 3.595703 | 0.389002 | -0.027547 |
| 8 | 2.961897 | 1.121013 | -0.870065 |
| 6 | -0.892054 | -1.319469 | 2.211413 |
| 8 | -0.367466 | -1.833703 | 1.148422 |
| 6 | 5.075142 | 0.631981 | 0.054111 |
| 1 | 5.498289 | 0.757333 | -0.947867 |
| 1 | 5.246401 | 1.570087 | 0.596699 |
| 1 | 5.573880 | -0.182118 | 0.585535 |
| 6 | -2.324153 | -1.726661 | 2.470289 |
| 1 | -2.582090 | -1.578774 | 3.523089 |
| 1 | -2.979082 | -1.087575 | 1.861016 |
| 1 | -2.502514 | -2.765020 | 2.170972 |
| 1 | 2.069525 | 0.234222 | -2.476776 |
| 6 | -0.840724 | -0.712405 | -1.698373 |

| | | | |
|---|---|---|---|
| 6 | -2.129364 | -0.253464 | -1.377895 |
| 6 | -0.627461 | -2.088049 | -1.885291 |
| 6 | -3.173498 | -1.155679 | -1.254020 |
| 1 | -2.317589 | 0.809043 | -1.247240 |
| 6 | -1.673966 | -2.983449 | -1.748349 |
| 1 | 0.373727 | -2.443720 | -2.115674 |
| 6 | -2.947416 | -2.518833 | -1.432272 |
| 1 | -4.171626 | -0.793339 | -1.016216 |
| 1 | -1.495783 | -4.048664 | -1.877723 |
| 1 | -3.769456 | -3.224081 | -1.321125 |
| 1 | 1.671399 | 1.247371 | -0.814637 |

**Q**

E= -615.4422683 a.u.

| | | | |
|---|---|---|---|
| 6 | -0.702918 | 1.618627 | 0.021626 |
| 8 | -1.474350 | 2.741941 | -0.026954 |
| 6 | 0.644641 | 1.694330 | 0.034723 |
| 1 | 1.068559 | 2.700639 | 0.125367 |
| 6 | 1.639445 | 0.625008 | -0.072261 |
| 6 | 1.450047 | -0.526672 | -0.851032 |
| 6 | 2.869630 | 0.778247 | 0.582040 |
| 6 | 2.437529 | -1.498354 | -0.936925 |
| 1 | 0.518456 | -0.651214 | -1.401142 |
| 6 | 3.860558 | -0.191509 | 0.491783 |
| 1 | 3.041647 | 1.676354 | 1.176832 |
| 6 | 3.646733 | -1.340111 | -0.263468 |
| 1 | 2.265655 | -2.383194 | -1.548331 |
| 1 | 4.805562 | -0.048466 | 1.014144 |
| 1 | 4.421065 | -2.101710 | -0.339096 |
| 1 | -0.897534 | 3.506556 | -0.172385 |
| 6 | -1.541245 | 0.408366 | 0.089567 |
| 6 | -1.186965 | -0.669678 | 0.908085 |
| 6 | -2.740817 | 0.350269 | -0.627050 |
| 6 | -1.998882 | -1.792856 | 0.981814 |
| 1 | -0.269346 | -0.618214 | 1.491531 |
| 6 | -3.550632 | -0.776991 | -0.554253 |
| 1 | -3.031837 | 1.198948 | -1.242524 |
| 6 | -3.180607 | -1.852564 | 0.246602 |
| 1 | -1.712753 | -2.624126 | 1.623992 |
| 1 | -4.477438 | -0.813070 | -1.124658 |
| 1 | -3.816333 | -2.734698 | 0.304397 |

**TS14**

E= -1268.4081333 a.u.

| | | | |
|---|---|---|---|
| 6 | 0.568500 | 0.361475 | -0.737360 |
| 8 | -0.711256 | 0.149370 | -1.185570 |
| 6 | 1.478890 | -0.593321 | -1.023698 |
| 1 | 1.108712 | -1.394766 | -1.665568 |
| 6 | 2.861967 | -0.728005 | -0.579667 |
| 6 | 3.357304 | -0.191569 | 0.619710 |
| 6 | 3.736098 | -1.488575 | -1.371393 |
| 6 | 4.681022 | -0.383848 | 0.988079 |
| 1 | 2.691790 | 0.366179 | 1.275867 |
| 6 | 5.061537 | -1.677004 | -1.004039 |
| 1 | 3.357949 | -1.930399 | -2.293870 |
| 6 | 5.542153 | -1.120345 | 0.177127 |
| 1 | 5.042866 | 0.035915 | 1.925555 |
| 1 | 5.720061 | -2.266596 | -1.640028 |
| 1 | 6.579594 | -1.269330 | 0.471685 |
| 6 | 0.774333 | 1.624863 | -0.002708 |
| 6 | 1.840187 | 2.472783 | -0.321646 |
| 6 | -0.118660 | 2.007787 | 1.003645 |
| 6 | 2.020773 | 3.664591 | 0.367406 |
| 1 | 2.526894 | 2.186047 | -1.117026 |
| 6 | 0.066568 | 3.197810 | 1.696480 |
| 1 | -0.963540 | 1.363834 | 1.252867 |
| 6 | 1.137590 | 4.028035 | 1.380980 |
| 1 | 2.851960 | 4.317379 | 0.106607 |
| 1 | -0.630044 | 3.478747 | 2.484421 |
| 1 | 1.280061 | 4.963553 | 1.919248 |
| 29 | -1.962973 | -0.952618 | -0.116846 |
| 6 | -1.814898 | -3.116427 | 0.769274 |
| 8 | -0.835903 | -2.556526 | 0.177931 |
| 8 | -2.890504 | -2.456996 | 0.875133 |
| 6 | -1.684808 | -4.487802 | 1.338181 |
| 1 | -2.639400 | -5.018043 | 1.270530 |

| | | | |
|---|---|---|---|
| 1 | -0.894022 | -5.042345 | 0.825380 |
| 1 | -1.418960 | -4.408955 | 2.399598 |
| 6 | -3.329611 | 1.490033 | -0.705191 |
| 8 | -3.353398 | 0.364861 | -0.101310 |
| 8 | -2.358775 | 1.939170 | -1.358387 |
| 6 | -4.586014 | 2.307422 | -0.604125 |
| 1 | -5.401072 | 1.779508 | -1.113116 |
| 1 | -4.878821 | 2.408729 | 0.446629 |
| 1 | -4.445227 | 3.291814 | -1.057278 |
| 1 | -1.321495 | 1.038186 | -1.311665 |

**R**

E= -1039.4330842 a.u.

| | | | |
|---|---|---|---|
| 6 | -0.541001 | -0.757141 | -0.574149 |
| 8 | 0.491033 | -1.480031 | -0.697962 |
| 6 | -0.433288 | 0.644787 | -0.846148 |
| 1 | 0.380475 | 0.887111 | -1.538568 |
| 6 | -1.151231 | 1.749650 | -0.299312 |
| 6 | -1.982707 | 1.664789 | 0.843671 |
| 6 | -0.969877 | 3.021439 | -0.892747 |
| 6 | -2.616248 | 2.790239 | 1.337892 |
| 1 | -2.105903 | 0.708971 | 1.348748 |
| 6 | -1.614098 | 4.140313 | -0.397108 |
| 1 | -0.312531 | 3.104255 | -1.758072 |
| 6 | -2.444142 | 4.030450 | 0.719314 |
| 1 | -3.244071 | 2.708292 | 2.223133 |
| 1 | -1.466913 | 5.106958 | -0.875065 |
| 1 | -2.945074 | 4.911701 | 1.115640 |
| 6 | -1.802291 | -1.433439 | -0.216739 |
| 6 | -3.043042 | -0.950808 | -0.650566 |
| 6 | -1.741540 | -2.631733 | 0.503949 |
| 6 | -4.204812 | -1.649836 | -0.354309 |
| 1 | -3.089042 | -0.034697 | -1.237749 |
| 6 | -2.906567 | -3.320115 | 0.810668 |
| 1 | -0.769153 | -3.004329 | 0.819154 |
| 6 | -4.138146 | -2.830858 | 0.381490 |
| 1 | -5.165291 | -1.276976 | -0.704928 |
| 1 | -2.856020 | -4.243981 | 1.383638 |
| 1 | -5.050852 | -3.375491 | 0.617597 |
| 29 | 2.179988 | -0.668156 | -0.506632 |
| 6 | 4.276368 | -0.092740 | 0.515322 |
| 8 | 3.845291 | 0.295105 | -0.629439 |
| 8 | 3.600062 | -0.843294 | 1.248882 |
| 6 | 5.639582 | 0.387457 | 0.931455 |
| 1 | 5.686922 | 1.480191 | 0.863143 |
| 1 | 5.873308 | 0.064270 | 1.949107 |
| 1 | 6.391639 | -0.008707 | 0.238606 |

**TS15**

E= -1612.6944559 a.u.

| | | | |
|---|---|---|---|
| 6 | -1.811273 | -0.809022 | -0.153357 |
| 8 | -0.733912 | -1.429331 | 0.024848 |
| 6 | -1.786883 | 0.629093 | -0.262556 |
| 1 | -0.823793 | 1.023335 | -0.607194 |
| 6 | -2.767920 | 1.587213 | 0.111601 |
| 6 | -3.934164 | 1.300053 | 0.866227 |
| 6 | -2.519401 | 2.940947 | -0.231767 |
| 6 | -4.803091 | 2.312205 | 1.229109 |
| 1 | -4.135065 | 0.278319 | 1.181183 |
| 6 | -3.399809 | 3.944238 | 0.126637 |
| 1 | -1.617455 | 3.172769 | -0.798424 |
| 6 | -4.548000 | 3.635123 | 0.858519 |
| 1 | -5.687829 | 2.074596 | 1.816876 |
| 1 | -3.193170 | 4.974626 | -0.156053 |
| 1 | -5.238297 | 4.424695 | 1.149581 |
| 6 | -3.042754 | -1.612446 | -0.298810 |
| 6 | -4.100318 | -1.182296 | -1.109334 |
| 6 | -3.111363 | -2.867858 | 0.316110 |
| 6 | -5.214319 | -1.990667 | -1.288859 |
| 1 | -4.035102 | -0.219474 | -1.614090 |
| 6 | -4.235212 | -3.664421 | 0.150761 |
| 1 | -2.272608 | -3.200562 | 0.924045 |
| 6 | -5.286383 | -3.227510 | -0.652731 |
| 1 | -6.027471 | -1.658230 | -1.931134 |
| 1 | -4.291209 | -4.633192 | 0.643389 |
| 1 | -6.163636 | -3.857503 | -0.789118 |

| | | | |
|---|---|---|---|
| 29 | 1.044820 | -0.703941 | 0.288464 |
| 6 | 2.160457 | 1.906429 | -0.478994 |
| 8 | 1.259118 | 1.119926 | -0.850261 |
| 8 | 3.354632 | 1.574061 | -0.190606 |
| 6 | 1.827400 | 3.371028 | -0.349468 |
| 1 | 1.044475 | 3.497388 | 0.409337 |
| 1 | 2.703489 | 3.961536 | -0.069593 |
| 1 | 1.421058 | 3.737062 | -1.300018 |
| 14 | 4.183709 | -0.154512 | -0.501020 |
| 6 | 5.761580 | 0.318083 | 0.398158 |
| 1 | 6.622049 | -0.075174 | -0.160723 |
| 1 | 5.873619 | 1.403107 | 0.496498 |
| 1 | 5.804332 | -0.125585 | 1.402542 |
| 6 | 4.309059 | -2.053921 | -0.763022 |
| 1 | 4.481952 | -2.630501 | 0.156229 |
| 1 | 3.395193 | -2.447319 | -1.234941 |
| 1 | 5.141113 | -2.266664 | -1.450866 |
| 6 | 4.137255 | 0.313028 | -2.346829 |
| 1 | 3.109066 | 0.216932 | -2.724856 |
| 1 | 4.454997 | 1.348330 | -2.521973 |
| 1 | 4.769154 | -0.361694 | -2.938950 |
| 7 | 2.848555 | -0.585761 | 0.986591 |
| 7 | 3.277922 | -1.227692 | 1.931416 |
| 7 | 3.722893 | -1.796887 | 2.820115 |

**S**

E= -975.1679621 a.u.

| | | | |
|---|---|---|---|
| 6 | -0.324589 | -0.810439 | -0.234174 |
| 8 | 0.597631 | -1.663874 | -0.106768 |
| 6 | 0.025718 | 0.554411 | -0.513142 |
| 1 | 1.001112 | 0.654938 | -1.000599 |
| 6 | -0.627276 | 1.769879 | -0.169529 |
| 6 | -1.722475 | 1.866193 | 0.726132 |
| 6 | -0.102318 | 2.972904 | -0.705421 |
| 6 | -2.273508 | 3.095999 | 1.031986 |
| 1 | -2.116901 | 0.965689 | 1.191160 |
| 6 | -0.665131 | 4.197269 | -0.399426 |
| 1 | 0.757786 | 2.916497 | -1.372057 |
| 6 | -1.757182 | 4.265587 | 0.467599 |
| 1 | -3.108890 | 3.152072 | 1.727214 |
| 1 | -0.250806 | 5.107152 | -0.828746 |
| 1 | -2.197766 | 5.229615 | 0.714535 |
| 6 | -1.711989 | -1.301371 | -0.146317 |
| 6 | -2.756942 | -0.678999 | -0.841192 |
| 6 | -1.968411 | -2.469053 | 0.582802 |
| 6 | -4.039453 | -1.206973 | -0.790528 |
| 1 | -2.555535 | 0.210808 | -1.435760 |
| 6 | -3.254707 | -2.984802 | 0.643479 |
| 1 | -1.144341 | -2.956902 | 1.098899 |
| 6 | -4.290706 | -2.354628 | -0.042314 |
| 1 | -4.845282 | -0.725338 | -1.340797 |
| 1 | -3.452233 | -3.884169 | 1.223367 |
| 1 | -5.298466 | -2.764006 | 0.001506 |
| 29 | 2.420584 | -1.276256 | 0.015021 |
| 7 | 4.213136 | -0.984132 | 0.139707 |
| 7 | 4.794301 | 0.075343 | 0.129732 |
| 7 | 5.427871 | 1.040247 | 0.127715 |

**TS16**

E= -975.1597696 a.u.

| | | | |
|---|---|---|---|
| 6 | -1.005645 | 0.331323 | 0.406012 |
| 8 | -0.579538 | -0.232400 | 1.447645 |
| 6 | -0.033665 | 0.810110 | -0.555745 |
| 6 | 1.259564 | 1.368987 | -0.213467 |
| 6 | 1.694619 | 1.615449 | 1.113644 |
| 6 | 2.142961 | 1.696188 | -1.272805 |
| 6 | 2.943313 | 2.168849 | 1.349005 |
| 1 | 1.037849 | 1.368989 | 1.943958 |
| 6 | 3.384661 | 2.246769 | -1.022511 |
| 1 | 1.824383 | 1.500851 | -2.296779 |
| 6 | 3.793569 | 2.486650 | 0.291352 |
| 1 | 3.257394 | 2.355819 | 2.374058 |
| 1 | 4.044901 | 2.488785 | -1.852940 |
| 1 | 4.773472 | 2.917290 | 0.487447 |
| 6 | -2.452299 | 0.392774 | 0.126437 |
| 6 | -2.981101 | 1.226040 | -0.865098 |

| | | | |
|---|---|---|---|
| 6 | -3.314618 | -0.388911 | 0.903636 |
| 6 | -4.351623 | 1.267473 | -1.083910 |
| 1 | -2.320785 | 1.862420 | -1.452682 |
| 6 | -4.682677 | -0.347658 | 0.681836 |
| 1 | -2.885861 | -1.026245 | 1.673958 |
| 6 | -5.201514 | 0.478467 | -0.313315 |
| 1 | -4.759310 | 1.921428 | -1.852247 |
| 1 | -5.349160 | -0.962321 | 1.283781 |
| 1 | -6.275792 | 0.510119 | -0.487219 |
| 29 | 0.944813 | -0.981231 | 0.028849 |
| 7 | 2.003062 | -2.437959 | -0.334402 |
| 7 | 1.732793 | -3.614666 | -0.370297 |
| 7 | 1.557860 | -4.753474 | -0.425554 |
| 1 | -0.339638 | 0.905403 | -1.597760 |

**T**

E= -975.1546338 a.u.

| | | | |
|---|---|---|---|
| 6 | 1.044506 | 0.853263 | -1.214167 |
| 8 | 0.906118 | 1.947640 | -1.744462 |
| 6 | -0.012418 | -0.165770 | -1.421486 |
| 6 | -0.433670 | -1.255431 | -0.583368 |
| 6 | -0.093407 | -1.373906 | 0.802939 |
| 6 | -1.355490 | -2.212831 | -1.113857 |
| 6 | -0.620127 | -2.394774 | 1.573200 |
| 1 | 0.588675 | -0.650334 | 1.245656 |
| 6 | -1.865190 | -3.225899 | -0.327474 |
| 1 | -1.640753 | -2.128593 | -2.162494 |
| 6 | -1.498404 | -3.328521 | 1.018461 |
| 1 | -0.350899 | -2.460288 | 2.625327 |
| 1 | -2.560336 | -3.943860 | -0.757908 |
| 1 | -1.908976 | -4.124299 | 1.636104 |
| 6 | 2.267766 | 0.555131 | -0.417647 |
| 6 | 2.805967 | -0.731588 | -0.317488 |
| 6 | 2.938905 | 1.630596 | 0.171646 |
| 6 | 3.993146 | -0.939748 | 0.373993 |
| 1 | 2.304858 | -1.570077 | -0.800630 |
| 6 | 4.112161 | 1.417937 | 0.881452 |
| 1 | 2.518812 | 2.627837 | 0.055173 |
| 6 | 4.640405 | 0.132445 | 0.982126 |
| 1 | 4.416540 | -1.940488 | 0.437635 |
| 1 | 4.621996 | 2.255826 | 1.353384 |
| 1 | 5.565648 | -0.033528 | 1.531541 |
| 29 | -1.666058 | 0.459825 | -0.372356 |
| 7 | -3.073663 | 1.510118 | 0.108264 |
| 7 | -3.194458 | 2.364444 | 0.953555 |
| 7 | -3.392299 | 3.187445 | 1.735416 |
| 1 | -0.410788 | -0.147718 | -2.440386 |

**U**

E= -1204.162149 a.u.

| | | | |
|---|---|---|---|
| 6 | -1.190621 | -1.452719 | -0.521197 |
| 8 | -0.913123 | -1.770519 | -1.677609 |
| 6 | -0.180943 | -1.340145 | 0.535023 |
| 6 | 1.219069 | -1.643557 | 0.398692 |
| 6 | 1.876076 | -1.874642 | -0.851759 |
| 6 | 2.035849 | -1.595479 | 1.573506 |
| 6 | 3.251656 | -2.004294 | -0.901940 |
| 1 | 1.264165 | -1.934744 | -1.746270 |
| 6 | 3.406569 | -1.731704 | 1.498234 |
| 1 | 1.548850 | -1.433828 | 2.535928 |
| 6 | 4.025206 | -1.924510 | 0.258711 |
| 1 | 3.737255 | -2.153184 | -1.864253 |
| 1 | 4.006931 | -1.676030 | 2.403897 |
| 1 | 5.108261 | -2.000879 | 0.196358 |
| 6 | -2.609383 | -1.167146 | -0.149408 |
| 6 | -2.975487 | -0.424979 | 0.977802 |
| 6 | -3.607889 | -1.651780 | -0.999355 |
| 6 | -4.316244 | -0.182851 | 1.252715 |
| 1 | -2.210989 | 0.008500 | 1.620054 |
| 6 | -4.946799 | -1.420984 | -0.717680 |
| 1 | -3.304568 | -2.211998 | -1.881583 |
| 6 | -5.303582 | -0.686512 | 0.410837 |
| 1 | -4.591564 | 0.404479 | 2.127368 |
| 1 | -5.716538 | -1.812088 | -1.380898 |
| 1 | -6.353750 | -0.501360 | 0.631920 |
| 29 | 0.798764 | 0.447182 | 0.142922 |

| | | | |
|---|---|---|---|
| 7 | 2.219169 | 1.696334 | -0.256120 |
| 7 | 3.383182 | 1.409960 | -0.420319 |
| 7 | 4.496424 | 1.163917 | -0.578466 |
| 1 | -0.547365 | -1.277115 | 1.561152 |
| 6 | -0.683919 | 3.015910 | -0.067134 |
| 8 | 0.403742 | 3.650118 | -0.409579 |
| 8 | -0.741713 | 1.817486 | 0.224333 |
| 6 | -1.901207 | 3.883074 | -0.049364 |
| 1 | -2.783327 | 3.292644 | 0.208063 |
| 1 | -1.764211 | 4.692658 | 0.676858 |
| 1 | -2.033998 | 4.351030 | -1.031307 |
| 1 | 1.203932 | 3.029389 | -0.400957 |

**TS17**

E= -1204.1527655 a.u.

| | | | |
|---|---|---|---|
| 6 | -1.335847 | -1.529903 | -0.416519 |
| 8 | -1.046264 | -2.116926 | -1.458315 |
| 6 | -0.354126 | -1.277754 | 0.646655 |
| 6 | 1.038831 | -1.643248 | 0.609840 |
| 6 | 1.712245 | -2.134234 | -0.551701 |
| 6 | 1.827765 | -1.402893 | 1.778910 |
| 6 | 3.079668 | -2.344149 | -0.527254 |
| 1 | 1.119109 | -2.337383 | -1.438448 |
| 6 | 3.191000 | -1.622611 | 1.780038 |
| 1 | 1.326868 | -1.036465 | 2.675688 |
| 6 | 3.826666 | -2.093781 | 0.626745 |
| 1 | 3.576894 | -2.710743 | -1.423380 |
| 1 | 3.769569 | -1.424247 | 2.680034 |
| 1 | 4.902737 | -2.255187 | 0.624931 |
| 6 | -2.731337 | -1.066675 | -0.173631 |
| 6 | -3.042568 | -0.017804 | 0.698287 |
| 6 | -3.757527 | -1.705803 | -0.876536 |
| 6 | -4.366115 | 0.369607 | 0.873127 |
| 1 | -2.248949 | 0.539426 | 1.194393 |
| 6 | -5.078440 | -1.328097 | -0.686145 |
| 1 | -3.491567 | -2.504265 | -1.566530 |
| 6 | -5.384610 | -0.290798 | 0.192470 |
| 1 | -4.602673 | 1.197026 | 1.540004 |
| 1 | -5.874325 | -1.840282 | -1.224248 |
| 1 | -6.421034 | 0.008946 | 0.340563 |
| 29 | 0.702377 | 0.409594 | 0.047477 |
| 7 | 2.169331 | 1.321023 | -0.995529 |
| 7 | 3.376903 | 1.106339 | -1.004199 |
| 7 | 4.484921 | 0.845518 | -1.037579 |
| 1 | -0.751306 | -1.010232 | 1.627310 |
| 6 | -0.095637 | 3.163959 | 0.081007 |
| 8 | 0.949541 | 3.503860 | -0.521092 |
| 8 | -0.399898 | 1.982269 | 0.454201 |
| 6 | -1.122291 | 4.227536 | 0.379116 |
| 1 | -1.936035 | 4.142812 | -0.352273 |
| 1 | -1.557805 | 4.074381 | 1.371921 |
| 1 | -0.682471 | 5.225301 | 0.300098 |
| 1 | 1.810879 | 2.368796 | -0.870570 |

**V**

E= -1204.1529235 a.u.

| | | | |
|---|---|---|---|
| 6 | -1.343381 | -1.533189 | -0.417461 |
| 8 | -1.066968 | -2.118336 | -1.463768 |
| 6 | -0.346838 | -1.280259 | 0.632493 |
| 6 | 1.044397 | -1.649745 | 0.578182 |
| 6 | 1.705756 | -2.126788 | -0.596088 |
| 6 | 1.844927 | -1.428749 | 1.743196 |
| 6 | 3.073347 | -2.338635 | -0.587960 |
| 1 | 1.104013 | -2.317294 | -1.479708 |
| 6 | 3.207132 | -1.652087 | 1.728789 |
| 1 | 1.353455 | -1.072850 | 2.649373 |
| 6 | 3.831562 | -2.107023 | 0.562503 |
| 1 | 3.561208 | -2.693281 | -1.493986 |
| 1 | 3.794228 | -1.469905 | 2.626683 |
| 1 | 4.907253 | -2.270465 | 0.548389 |
| 6 | -2.735643 | -1.070086 | -0.156451 |
| 6 | -3.034070 | -0.014647 | 0.711989 |
| 6 | -3.771590 | -1.712106 | -0.841873 |
| 6 | -4.354339 | 0.378335 | 0.898801 |
| 1 | -2.233175 | 0.544685 | 1.193412 |
| 6 | -5.089356 | -1.329897 | -0.638127 |

| | | | |
|---|---|---|---|
| 1 | -3.515878 | -2.515401 | -1.530155 |
| 6 | -5.382521 | -0.284523 | 0.235297 |
| 1 | -4.580440 | 1.211850 | 1.561860 |
| 1 | -5.892738 | -1.844204 | -1.162928 |
| 1 | -6.416362 | 0.019477 | 0.392572 |
| 29 | 0.698283 | 0.404587 | 0.020559 |
| 7 | 2.241398 | 1.362304 | -0.845045 |
| 7 | 3.448545 | 1.153278 | -0.855513 |
| 7 | 4.558340 | 0.899833 | -0.884594 |
| 1 | -0.731486 | -1.017799 | 1.619655 |
| 6 | -0.146060 | 3.150174 | 0.014733 |
| 8 | 0.939303 | 3.522821 | -0.487059 |
| 8 | -0.458735 | 1.954327 | 0.333656 |
| 6 | -1.195084 | 4.193683 | 0.308782 |
| 1 | -2.193595 | 3.797652 | 0.095415 |
| 1 | -1.160525 | 4.442304 | 1.377204 |
| 1 | -1.007901 | 5.104576 | -0.266148 |
| 1 | 1.865514 | 2.402474 | -0.755232 |

**W**

E= -1204.1540171 a.u.

| | | | |
|---|---|---|---|
| 6 | -1.155121 | 1.355868 | 0.080424 |
| 8 | -0.981075 | 2.073679 | 1.083548 |
| 6 | -0.068721 | 0.923063 | -0.780937 |
| 6 | 1.268870 | 1.502035 | -0.820717 |
| 6 | 1.741003 | 2.497346 | 0.061276 |
| 6 | 2.160310 | 1.007402 | -1.800140 |
| 6 | 3.040969 | 2.967545 | -0.044179 |
| 1 | 1.061566 | 2.903348 | 0.805282 |
| 6 | 3.460045 | 1.477391 | -1.890192 |
| 1 | 1.807343 | 0.234832 | -2.484796 |
| 6 | 3.909021 | 2.461166 | -1.010578 |
| 1 | 3.384014 | 3.744538 | 0.637444 |
| 1 | 4.128048 | 1.077194 | -2.650932 |
| 1 | 4.928863 | 2.835218 | -1.081143 |
| 6 | -2.530836 | 0.862566 | -0.222336 |
| 6 | -2.789686 | -0.251445 | -1.031400 |
| 6 | -3.603420 | 1.538146 | 0.369607 |
| 6 | -4.097720 | -0.668588 | -1.247711 |
| 1 | -1.973709 | -0.824047 | -1.471249 |
| 6 | -4.908819 | 1.129852 | 0.137805 |
| 1 | -3.383951 | 2.390034 | 1.009729 |
| 6 | -5.158567 | 0.024380 | -0.672365 |
| 1 | -4.288479 | -1.542867 | -1.867430 |
| 1 | -5.736232 | 1.670652 | 0.594132 |
| 1 | -6.182272 | -0.300817 | -0.851080 |
| 29 | 0.556490 | -0.793931 | 0.220930 |
| 7 | 0.478902 | 0.005697 | 2.091391 |
| 7 | 0.852955 | -0.538635 | 3.136858 |
| 7 | 1.235927 | -1.119036 | 4.032092 |
| 1 | -0.362471 | 0.426007 | -1.707632 |
| 6 | 1.039636 | -2.982291 | -0.578126 |
| 8 | 1.423020 | -2.662603 | 0.580547 |
| 8 | 0.416105 | -2.137115 | -1.300312 |
| 6 | 1.293731 | -4.354119 | -1.124776 |
| 1 | 0.336449 | -4.869600 | -1.267720 |
| 1 | 1.767933 | -4.278703 | -2.109624 |
| 1 | 1.923310 | -4.935619 | -0.446430 |
| 1 | 0.008320 | 0.924029 | 2.197887 |

**TS18**

E= -1204.105778 a.u

| | | | |
|---|---|---|---|
| 6 | 0.337564 | 2.010408 | 0.394271 |
| 8 | -0.126939 | 3.130344 | 0.207973 |
| 6 | -0.526641 | 0.813255 | 0.507213 |
| 6 | -1.956847 | 0.814550 | 0.701312 |
| 6 | -2.793313 | 1.926968 | 0.478991 |
| 6 | -2.534511 | -0.413542 | 1.091264 |
| 6 | -4.165755 | 1.795322 | 0.620628 |
| 1 | -2.346865 | 2.873619 | 0.190677 |
| 6 | -3.907234 | -0.532635 | 1.223401 |
| 1 | -1.876930 | -1.264488 | 1.281998 |
| 6 | -4.726150 | 0.569897 | 0.979129 |
| 1 | -4.809669 | 2.654262 | 0.440864 |
| 1 | -4.344767 | -1.484534 | 1.518192 |
| 1 | -5.806514 | 0.475321 | 1.076375 |

| | | | |
|---|---|---|---|
| 6 | 1.813944 | 1.793117 | 0.414832 |
| 6 | 2.423101 | 0.566746 | 0.722035 |
| 6 | 2.618920 | 2.893197 | 0.090153 |
| 6 | 3.809225 | 0.454496 | 0.691675 |
| 1 | 1.840357 | -0.311307 | 1.004973 |
| 6 | 3.999585 | 2.774233 | 0.059881 |
| 1 | 2.127967 | 3.837789 | -0.135571 |
| 6 | 4.597576 | 1.551243 | 0.358841 |
| 1 | 4.273441 | -0.499467 | 0.934586 |
| 1 | 4.613985 | 3.635325 | -0.197118 |
| 1 | 5.681832 | 1.454552 | 0.335460 |
| 29 | 0.318689 | -1.489135 | -1.213318 |
| 7 | -0.309058 | 0.308864 | -1.518428 |
| 7 | -1.395698 | 0.381222 | -2.312122 |
| 7 | -2.550069 | 0.315472 | -2.283379 |
| 1 | -0.051244 | -0.102498 | 0.861983 |
| 6 | 0.848682 | -3.170784 | 0.629779 |
| 8 | 0.897613 | -3.161230 | -0.659106 |
| 8 | 0.497439 | -2.202843 | 1.324605 |
| 6 | 1.260849 | -4.474404 | 1.266374 |
| 1 | 2.291751 | -4.715023 | 0.980762 |
| 1 | 1.181292 | -4.419294 | 2.354995 |
| 1 | 0.630084 | -5.286511 | 0.886572 |
| 1 | 0.398219 | 0.935710 | -1.917479 |

**X**

E= -1094.7524545 a.u

| | | | |
|---|---|---|---|
| 6 | 1.819953 | -1.058155 | -0.664572 |
| 8 | 1.755191 | -1.669858 | -1.717930 |
| 6 | 0.522457 | -0.549412 | -0.025351 |
| 6 | 0.408866 | 0.961364 | -0.158412 |
| 6 | 0.684099 | 1.575409 | -1.380836 |
| 6 | -0.048689 | 1.729897 | 0.911239 |
| 6 | 0.523437 | 2.948728 | -1.521743 |
| 1 | 1.018182 | 0.971425 | -2.225342 |
| 6 | -0.212708 | 3.103862 | 0.767699 |
| 1 | -0.280201 | 1.244322 | 1.861485 |
| 6 | 0.077423 | 3.714798 | -0.448131 |
| 1 | 0.742819 | 3.423142 | -2.476663 |
| 1 | -0.569442 | 3.697413 | 1.607515 |
| 1 | -0.049976 | 4.789786 | -0.561854 |
| 6 | 3.116829 | -0.791409 | -0.000020 |
| 6 | 3.227617 | -0.052662 | 1.182988 |
| 6 | 4.270672 | -1.322808 | -0.588058 |
| 6 | 4.471795 | 0.148759 | 1.766485 |
| 1 | 2.345902 | 0.385690 | 1.647353 |
| 6 | 5.511444 | -1.123297 | -0.002797 |
| 1 | 4.163957 | -1.894450 | -1.507637 |
| 6 | 5.612643 | -0.387184 | 1.176049 |
| 1 | 4.551277 | 0.727701 | 2.684489 |
| 1 | 6.404533 | -1.541583 | -0.463307 |
| 1 | 6.586780 | -0.230087 | 1.636546 |
| 29 | -2.357820 | -0.906943 | -0.159426 |
| 7 | -0.622694 | -1.166919 | -0.642716 |
| 1 | 0.529693 | -0.799951 | 1.049931 |
| 6 | -4.587855 | -0.494803 | 0.438497 |
| 8 | -4.009095 | 0.266781 | -0.389456 |
| 8 | -3.954569 | -1.474828 | 0.937095 |
| 6 | -6.006597 | -0.242770 | 0.847903 |
| 1 | -6.584843 | -1.169970 | 0.771694 |
| 1 | -6.029018 | 0.064339 | 1.900492 |
| 1 | -6.459284 | 0.539114 | 0.232810 |
| 1 | -0.315262 | -1.675761 | -1.478462 |

**Y**

E= -1648.517605 a.u

| | | | |
|---|---|---|---|
| 6 | -0.278413 | 0.267417 | 0.342573 |
| 6 | -1.711276 | 0.086835 | -0.160795 |
| 6 | 0.006674 | -0.162329 | 1.719174 |
| 6 | -0.788145 | 0.291703 | 2.775860 |
| 6 | 1.043324 | -1.068065 | 1.960114 |
| 6 | -0.528397 | -0.134668 | 4.071633 |
| 1 | -1.586064 | 1.011863 | 2.593619 |
| 6 | 1.280933 | -1.506219 | 3.256278 |
| 1 | 1.636884 | -1.442170 | 1.124157 |
| 6 | 0.502988 | -1.038560 | 4.311134 |

| | | | |
|---|---|---|---|
| 1 | -1.131948 | 0.239617 | 4.896415 |
| 1 | 2.082048 | -2.219192 | 3.440954 |
| 1 | 0.699854 | -1.380245 | 5.326071 |
| 6 | -1.899307 | -1.416738 | -0.296080 |
| 6 | -1.252819 | -2.104069 | -1.324564 |
| 6 | -2.646836 | -2.128734 | 0.641353 |
| 6 | -1.370005 | -3.484900 | -1.422577 |
| 1 | -0.657065 | -1.551595 | -2.050702 |
| 6 | -2.764730 | -3.511202 | 0.540859 |
| 1 | -3.130973 | -1.596488 | 1.461962 |
| 6 | -2.126711 | -4.190896 | -0.491397 |
| 1 | -0.858680 | -4.012522 | -2.225756 |
| 1 | -3.351001 | -4.058389 | 1.276925 |
| 1 | -2.213591 | -5.273246 | -0.567371 |
| 29 | 2.514818 | 0.783918 | -0.364581 |
| 6 | 2.559073 | -1.349550 | -1.893828 |
| 8 | 2.510561 | -0.061861 | -2.064289 |
| 8 | 2.509230 | -1.906779 | -0.801839 |
| 6 | 2.685726 | -2.121599 | -3.186662 |
| 1 | 2.504086 | -3.184421 | -3.003262 |
| 1 | 1.986785 | -1.736682 | -3.937773 |
| 1 | 3.697444 | -1.991781 | -3.588972 |
| 7 | -1.844832 | 0.762245 | -1.430947 |
| 1 | -2.403034 | 0.466326 | 0.610875 |
| 7 | 0.613272 | 0.658087 | -0.483264 |
| 1 | 0.240613 | 0.848618 | -1.421042 |
| 6 | -2.892600 | 1.403692 | -1.765645 |
| 6 | -4.184574 | 1.579272 | -1.078683 |
| 6 | -4.821215 | 2.819672 | -1.207473 |
| 6 | -4.819207 | 0.559380 | -0.360578 |
| 6 | -6.041522 | 3.054718 | -0.589625 |
| 1 | -4.340427 | 3.606240 | -1.789871 |
| 6 | -6.052607 | 0.789475 | 0.237738 |
| 1 | -4.368456 | -0.430949 | -0.312164 |
| 6 | -6.658818 | 2.038042 | 0.134757 |
| 1 | -6.519168 | 4.028209 | -0.683148 |
| 1 | -6.547190 | -0.014324 | 0.780040 |
| 1 | -7.623091 | 2.215192 | 0.607987 |
| 8 | 2.366792 | 1.716392 | 1.148776 |
| 1 | 3.188941 | 2.254963 | 1.175503 |
| 1 | -2.820663 | 1.944069 | -2.720640 |
| 6 | 5.148549 | 1.686513 | 0.036344 |
| 8 | 4.829315 | 2.736411 | 0.575376 |
| 8 | 4.345063 | 0.750313 | -0.391604 |
| 6 | 6.592142 | 1.318760 | -0.226698 |
| 1 | 6.820579 | 0.353112 | 0.237497 |
| 1 | 6.756130 | 1.208748 | -1.304397 |
| 1 | 7.248160 | 2.095598 | 0.174783 |

**TS19**

E= -1648.4743265 a.u

| | | | |
|---|---|---|---|
| 6 | 0.577245 | 1.103294 | -0.959366 |
| 6 | 1.613539 | 0.060244 | -0.938992 |
| 6 | 0.646118 | 2.311749 | -0.118413 |
| 6 | 1.811500 | 3.091103 | -0.091102 |
| 6 | -0.488641 | 2.751094 | 0.578508 |
| 6 | 1.847689 | 4.274296 | 0.633336 |
| 1 | 2.688374 | 2.783457 | -0.658188 |
| 6 | -0.435712 | 3.921816 | 1.322211 |
| 1 | -1.421447 | 2.189192 | 0.544080 |
| 6 | 0.728696 | 4.683549 | 1.353346 |
| 1 | 2.753354 | 4.878131 | 0.635134 |
| 1 | -1.317324 | 4.238745 | 1.875183 |
| 1 | 0.761813 | 5.604385 | 1.933899 |
| 6 | 2.990790 | 0.300694 | -0.417067 |
| 6 | 4.087403 | 0.319789 | -1.282481 |
| 6 | 3.198595 | 0.480708 | 0.955184 |
| 6 | 5.367056 | 0.548942 | -0.786956 |
| 1 | 3.925776 | 0.169090 | -2.348792 |
| 6 | 4.477257 | 0.704973 | 1.446604 |
| 1 | 2.343026 | 0.450583 | 1.631868 |
| 6 | 5.564684 | 0.745178 | 0.575975 |
| 1 | 6.213998 | 0.573375 | -1.470567 |
| 1 | 4.626915 | 0.847294 | 2.515408 |
| 1 | 6.566473 | 0.922300 | 0.963422 |
| 7 | 1.558262 | -0.814742 | -2.070836 |

| | | | |
|---|---|---|---|
| 7 | -0.569322 | 0.837587 | -1.571248 |
| 1 | -0.427041 | 0.058474 | -2.226863 |
| 6 | 1.407492 | -2.079224 | -1.999929 |
| 6 | 1.258911 | -2.958631 | -0.825318 |
| 6 | 0.238807 | -3.915719 | -0.860919 |
| 6 | 2.074931 | -2.863175 | 0.306355 |
| 6 | -0.005838 | -4.721329 | 0.243858 |
| 1 | -0.383439 | -4.002738 | -1.752314 |
| 6 | 1.846996 | -3.692466 | 1.398334 |
| 1 | 2.896054 | -2.148190 | 0.325839 |
| 6 | 0.798725 | -4.609261 | 1.375638 |
| 1 | -0.820428 | -5.442306 | 0.219667 |
| 1 | 2.490015 | -3.620555 | 2.273507 |
| 1 | 0.613941 | -5.246387 | 2.238586 |
| 1 | 1.326950 | -2.591533 | -2.969760 |
| 1 | 0.872082 | -0.457768 | -0.007904 |
| 29 | -1.801244 | -0.182499 | -0.340261 |
| 6 | -3.803972 | 1.074362 | -1.360119 |
| 8 | -3.114744 | 0.008286 | -1.651303 |
| 8 | -3.588555 | 1.781849 | -0.384233 |
| 6 | -4.908592 | 1.350273 | -2.353516 |
| 1 | -4.480382 | 1.501594 | -3.350988 |
| 1 | -5.581805 | 0.487823 | -2.414726 |
| 1 | -5.466595 | 2.239964 | -2.049858 |
| 8 | -0.307999 | -0.695397 | 0.620664 |
| 1 | -0.473879 | -1.466720 | 1.188752 |
| 6 | -3.133085 | -0.629730 | 1.898454 |
| 8 | -2.525073 | 0.333658 | 2.328281 |
| 8 | -2.924022 | -1.215323 | 0.743238 |
| 6 | -4.266812 | -1.289631 | 2.658287 |
| 1 | -4.239617 | -2.378658 | 2.552972 |
| 1 | -4.216382 | -1.000789 | 3.711791 |
| 1 | -5.216491 | -0.938203 | 2.237369 |

**Z**

E= -1572.161043 a.u

| | | | |
|---|---|---|---|
| 6 | 0.941629 | -0.155629 | -0.956902 |
| 6 | 1.687848 | -1.151960 | -0.216354 |
| 6 | 1.358960 | 1.257774 | -1.028475 |
| 6 | 2.039609 | 1.887012 | 0.020029 |
| 6 | 0.994079 | 2.013321 | -2.148617 |
| 6 | 2.347956 | 3.237957 | -0.048573 |
| 1 | 2.319342 | 1.316689 | 0.905235 |
| 6 | 1.304708 | 3.363907 | -2.216639 |
| 1 | 0.449165 | 1.524178 | -2.953501 |
| 6 | 1.981107 | 3.980460 | -1.167828 |
| 1 | 2.868959 | 3.717055 | 0.778751 |
| 1 | 1.014447 | 3.940510 | -3.093160 |
| 1 | 2.221492 | 5.041102 | -1.220801 |
| 6 | 3.142039 | -1.169399 | -0.091013 |
| 6 | 3.974506 | -0.463271 | -0.976120 |
| 6 | 3.732664 | -1.956368 | 0.912129 |
| 6 | 5.352310 | -0.529605 | -0.843033 |
| 1 | 3.534677 | 0.127708 | -1.776555 |
| 6 | 5.110946 | -2.006980 | 1.050245 |
| 1 | 3.092678 | -2.530573 | 1.580698 |
| 6 | 5.924144 | -1.292185 | 0.173737 |
| 1 | 5.986381 | 0.015080 | -1.539495 |
| 1 | 5.554683 | -2.611468 | 1.838828 |
| 1 | 7.006773 | -1.336802 | 0.277322 |
| 29 | -1.917023 | -0.019011 | -0.734874 |
| 6 | -3.088526 | -2.047311 | -1.739108 |
| 8 | -2.278694 | -1.976711 | -0.726113 |
| 8 | -3.346371 | -1.080069 | -2.455854 |
| 6 | -3.702489 | -3.406756 | -1.977802 |
| 1 | -4.321413 | -3.394469 | -2.878903 |
| 1 | -2.917362 | -4.166005 | -2.075805 |
| 1 | -4.318538 | -3.688431 | -1.115230 |
| 7 | 1.017462 | -2.233362 | 0.227491 |
| 7 | -0.166490 | -0.496871 | -1.593997 |
| 1 | -0.302592 | -1.511700 | -1.583078 |
| 6 | -0.021629 | -2.280782 | 0.981925 |
| 6 | -0.470256 | -1.239525 | 1.897173 |
| 6 | -1.833305 | -1.177533 | 2.218342 |
| 6 | 0.415187 | -0.290153 | 2.429456 |
| 6 | -2.308048 | -0.147106 | 3.018735 |

| | | | |
|---|---|---|---|
| 1 | -2.519279 | -1.889558 | 1.762267 |
| 6 | -0.062154 | 0.724206 | 3.241576 |
| 1 | 1.482940 | -0.372461 | 2.226277 |
| 6 | -1.425831 | 0.800876 | 3.527553 |
| 1 | -3.374756 | -0.068638 | 3.216408 |
| 1 | 0.626552 | 1.459186 | 3.653713 |
| 1 | -1.800419 | 1.607727 | 4.155745 |
| 1 | -0.615345 | -3.197969 | 0.943254 |
| 6 | -2.729553 | 1.886471 | 0.474471 |
| 8 | -1.559212 | 1.827321 | -0.025946 |
| 8 | -3.533563 | 0.930798 | 0.338356 |
| 6 | -3.138728 | 3.123971 | 1.221326 |
| 1 | -3.774071 | 3.742949 | 0.575795 |
| 1 | -3.734028 | 2.849092 | 2.099879 |
| 1 | -2.263740 | 3.710682 | 1.518292 |

**Za**

E= -919.2013504 a.u

| | | | |
|---|---|---|---|
| 6 | -0.995321 | -0.689613 | -1.165266 |
| 6 | -0.383720 | 0.539246 | -0.556939 |
| 6 | -1.791133 | -1.554219 | -0.255678 |
| 6 | -1.481634 | -1.615264 | 1.106359 |
| 6 | -2.851087 | -2.322280 | -0.747810 |
| 6 | -2.200364 | -2.451363 | 1.952582 |
| 1 | -0.664849 | -1.008262 | 1.497796 |
| 6 | -3.580026 | -3.143911 | 0.101233 |
| 1 | -3.125260 | -2.249972 | -1.801179 |
| 6 | -3.251245 | -3.214463 | 1.452913 |
| 1 | -1.943128 | -2.501344 | 3.009083 |
| 1 | -4.412799 | -3.726012 | -0.289604 |
| 1 | -3.822762 | -3.858809 | 2.118736 |
| 6 | -1.242353 | 1.664241 | -0.240327 |
| 6 | -2.603820 | 1.661095 | -0.595595 |
| 6 | -0.728450 | 2.795465 | 0.422825 |
| 6 | -3.418356 | 2.742728 | -0.295018 |
| 1 | -3.024101 | 0.805000 | -1.122719 |
| 6 | -1.546507 | 3.871784 | 0.719572 |
| 1 | 0.324852 | 2.800416 | 0.694273 |
| 6 | -2.896127 | 3.852724 | 0.364676 |
| 1 | -4.468744 | 2.721859 | -0.580910 |
| 1 | -1.131773 | 4.737883 | 1.233346 |
| 1 | -3.536117 | 4.701335 | 0.600628 |
| 7 | 0.914335 | 0.613835 | -0.271458 |
| 7 | -0.765411 | -0.919847 | -2.401763 |
| 1 | -1.197817 | -1.808491 | -2.681483 |
| 6 | 1.758005 | -0.368697 | -0.514160 |
| 6 | 3.154254 | -0.263966 | -0.175649 |
| 6 | 4.011587 | -1.345193 | -0.441523 |
| 6 | 3.690591 | 0.894123 | 0.417829 |
| 6 | 5.359578 | -1.275623 | -0.123410 |
| 1 | 3.600496 | -2.243307 | -0.904276 |
| 6 | 5.037039 | 0.959011 | 0.732789 |
| 1 | 3.021503 | 1.729257 | 0.616964 |
| 6 | 5.877796 | -0.123442 | 0.465314 |
| 1 | 6.012000 | -2.120956 | -0.336067 |
| 1 | 5.442727 | 1.860524 | 1.189713 |
| 1 | 6.936085 | -0.067048 | 0.714905 |
| 1 | 1.434975 | -1.304309 | -0.994955 |

**TS20**

E= -919.1802097 a.u

| | | | |
|---|---|---|---|
| 6 | 1.264159 | 0.361737 | 0.359351 |
| 6 | 1.492389 | -1.034671 | 0.056556 |
| 6 | 2.320874 | 1.392594 | 0.436313 |
| 6 | 3.528725 | 1.158990 | 1.104726 |
| 6 | 2.088736 | 2.656094 | -0.117747 |
| 6 | 4.480522 | 2.164591 | 1.206755 |
| 1 | 3.712705 | 0.182451 | 1.550591 |
| 6 | 3.047077 | 3.658910 | -0.023316 |
| 1 | 1.151998 | 2.837723 | -0.644811 |
| 6 | 4.245692 | 3.415142 | 0.639222 |
| 1 | 5.413025 | 1.971796 | 1.734710 |
| 1 | 2.857689 | 4.633488 | -0.470549 |
| 1 | 4.997005 | 4.199249 | 0.717314 |
| 6 | 2.719817 | -1.618430 | -0.488236 |
| 6 | 3.593993 | -0.899781 | -1.316893 |

| | | | |
|---|---|---|---|
| 6 | 3.005636 | -2.967476 | -0.229373 |
| 6 | 4.731583 | -1.502117 | -1.838354 |
| 1 | 3.371690 | 0.136088 | -1.567920 |
| 6 | 4.144539 | -3.564787 | -0.749214 |
| 1 | 2.311579 | -3.532990 | 0.389557 |
| 6 | 5.017343 | -2.834140 | -1.552486 |
| 1 | 5.394634 | -0.926268 | -2.482372 |
| 1 | 4.353142 | -4.610786 | -0.528226 |
| 1 | 5.910168 | -3.303609 | -1.962583 |
| 7 | 0.496263 | -1.832849 | 0.444884 |
| 7 | 0.023800 | 0.628566 | 0.698179 |
| 1 | -0.137458 | 1.540571 | 1.124991 |
| 6 | -0.699522 | -1.272609 | 0.591760 |
| 6 | -1.570383 | -1.617851 | 1.718830 |
| 6 | -2.903596 | -1.198177 | 1.711413 |
| 6 | -1.080522 | -2.333176 | 2.816150 |
| 6 | -3.737770 | -1.487497 | 2.782824 |
| 1 | -3.277237 | -0.635066 | 0.855054 |
| 6 | -1.917275 | -2.630266 | 3.882201 |
| 1 | -0.040560 | -2.655173 | 2.803630 |
| 6 | -3.245241 | -2.205986 | 3.869800 |
| 1 | -4.775140 | -1.157273 | 2.771109 |
| 1 | -1.535179 | -3.194690 | 4.731373 |
| 1 | -3.897796 | -2.437297 | 4.710283 |
| 1 | -1.229976 | -0.921486 | -0.303505 |

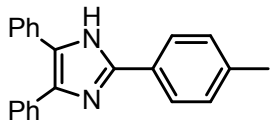
**Zb**

E= -919.221609 a.u

| | | | |
|---|---|---|---|
| 6 | 0.256496 | 0.673612 | -0.620982 |
| 6 | 0.351477 | -0.754941 | -0.645913 |
| 6 | 1.131493 | 1.713659 | -0.133927 |
| 6 | 2.060952 | 1.487103 | 0.899637 |
| 6 | 1.020168 | 3.019355 | -0.650598 |
| 6 | 2.851691 | 2.519614 | 1.378212 |
| 1 | 2.141449 | 0.495225 | 1.340360 |
| 6 | 1.814989 | 4.047657 | -0.164759 |
| 1 | 0.323871 | 3.209389 | -1.466793 |
| 6 | 2.736485 | 3.805505 | 0.850536 |
| 1 | 3.558901 | 2.322819 | 2.182509 |
| 1 | 1.718472 | 5.046367 | -0.588302 |
| 1 | 3.359189 | 4.612996 | 1.231340 |
| 6 | 1.523625 | -1.582752 | -0.312641 |
| 6 | 2.824273 | -1.191181 | -0.644819 |
| 6 | 1.322344 | -2.824812 | 0.296969 |
| 6 | 3.902209 | -2.018693 | -0.354627 |
| 1 | 2.987465 | -0.235824 | -1.142267 |
| 6 | 2.401450 | -3.647020 | 0.593577 |
| 1 | 0.303137 | -3.132817 | 0.525921 |
| 6 | 3.694776 | -3.245453 | 0.269952 |
| 1 | 4.909925 | -1.706456 | -0.624067 |
| 1 | 2.233082 | -4.608942 | 1.075408 |
| 1 | 4.541302 | -3.890387 | 0.500508 |
| 7 | -0.758812 | -1.330425 | -1.051847 |
| 7 | -0.974644 | 0.979353 | -1.170565 |
| 6 | -1.713830 | -0.291987 | -1.325820 |
| 6 | -2.925700 | -0.320507 | -0.417994 |
| 6 | -4.139450 | 0.191696 | -0.873314 |
| 6 | -2.828593 | -0.790061 | 0.891224 |
| 6 | -5.246355 | 0.239045 | -0.031642 |
| 1 | -4.216621 | 0.549182 | -1.901754 |
| 6 | -3.934716 | -0.746723 | 1.732031 |
| 1 | -1.883218 | -1.204867 | 1.239927 |
| 6 | -5.144564 | -0.231737 | 1.273477 |
| 1 | -6.191752 | 0.635511 | -0.398930 |
| 1 | -3.854304 | -1.122876 | 2.750846 |
| 1 | -6.010761 | -0.203693 | 1.932653 |
| 1 | -2.060255 | -0.385897 | -2.371266 |
| 1 | -1.480997 | 1.769507 | -0.780679 |

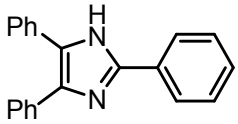
# IV. Analytical Data

2-(4-methylphenyl)-4,5-diphenyl-1*H*-imidazole (**3a**) [10]



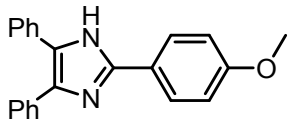
Starting from 1,2-diphenylethanone (0.4 mmol, 78.4 mg) and 4-methylbenzaldehyde (0.2 mmol, 24 μL), to give the product as a white solid, 51 mg, 82% yield, eluent: petroleum ether/ethyl acetate 8/1. $^1$H NMR (400 MHz, DMSO-$d_6$): δ 12.58 (br s, 1H), 7.97 (d, $J$ = 8.2 Hz, 2H), 7.54 (d, $J$ = 7.2 Hz, 2H), 7.49 (d, $J$ = 7.2 Hz, 2H), 7.45-7.42 (m, 2H), 7.38-7.35 (m, 1H), 7.32-7.27 (m, 4H), 7.23-7.20 (m, 1H), 2.35 (s, 3H); $^{13}$C NMR (125 MHz, DMSO-$d_6$): δ 145.6, 137.7, 136.9, 135.2, 131.1, 129.2, 128.6, 128.4, 128.1, 127.9, 127.6, 127.0, 126.4, 125.1, 20.8;

2, 4, 5-triphenyl-1*H*-imidazole (**3b**) [12]



Starting from 1,2-diphenylethanone (0.4 mmol, 78.4 mg) and benzaldehyde (0.2 mmol, 20.4 μL), to give the product as a white solid, 49 mg, 83% yield, eluent: petroleum ether/ethyl acetate 8/1. $^1$H NMR (400 MHz, DMSO-$d_6$): δ 12.68 (br s, 1H), 8.08 (d, $J$ = 7.4 Hz, 2H), 7.55 (d, $J$ = 7.4 Hz, 2H), 7.52-7.43 (m, 6H), 7.39-7.36 (m, 2H), 7.32-7.29 (m, 2H), 7.24-7.20 (m, 1H); $^{13}$C NMR (125 MHz, DMSO-$d_6$): δ 145.5, 137.1, 135.1, 131.0, 130.3, 128.6, 128.6, 128.4, 128.2, 128.1, 127.7, 127.0, 126.5, 125.2.

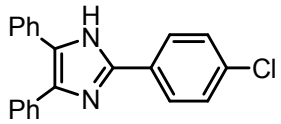
2-(4-methoxyphenyl)-4,5-diphenyl-1*H*-imidazole (**3c**) [14]



Starting from 1,2-diphenylethanone (0.4 mmol, 78.4 mg) and 4-methoxybenzaldehyde (0.2 mmol, 24.3 μL) to give the product as a white solid, 39 mg, 60% yield, eluent: petroleum ether/ethyl acetate 4/1. $^1$H NMR (400 MHz, DMSO-$d_6$): δ 12.50 (br s, 1H), 8.02 (d, $J$ = 8.8 Hz, 2H), 7.54 (d, $J$ = 7.3 Hz, 2H), 7.49 (d, $J$ =7.2 Hz, 2H), 7.45-7.41 (m, 2H), 7.38-7.34 (m, 1H), 7.31-7.28 (m, 2H), 7.23-7.19 (m, 1H), 7.04 (d, $J$ = 8.8 Hz, 2H), 3.82 (s, 3H); $^{13}$C NMR (125 MHz, DMSO-$d_6$): δ 159.4, 145.6, 136.7, 135.3, 131.2, 128.6, 128.3, 128.1, 127.6, 127.6, 127.0, 126.7, 126.3, 123.1, 114.1,

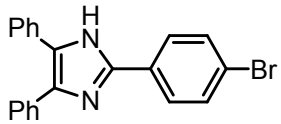
55.2.

2-(4-chlorophenyl)-4,5-diphenyl-1*H*-imidazole (**3d**) [12]



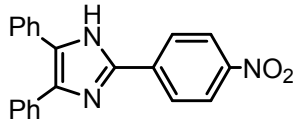

Starting from 1,2-diphenylethanone (0.4 mmol, 78.4 mg) and 4-chlorobenzaldehyde (0.2 mmol, 29 mg) to give the product as a white solid, 40 mg, 61% yield, eluent: petroleum ether/ethyl acetate 8/1. $^{1}$H NMR (400 MHz, DMSO-$d_6$): δ 12.77 (br s, 1H), 8.10 (d, $J$ = 8.4 Hz, 2H), 7.55-7.49 (m, 6H), 7.46-7.43 (m, 2H), 7.38 (d, $J$ = 6.6 Hz, 1H), 7.32- 7.29 (m, 2H), 7.23 (d, $J$ = 6.8, 1H); $^{13}$C NMR (125 MHz, DMSO-$d_6$): δ 144.9, 137.8, 135.5, 133.2, 131.4, 129.7, 129.2, 129.1, 129.0, 128.9, 128.7, 128.3, 127.5, 127.3, 127.1.

2-(4-bromophenyl)-4,5-diphenyl-1*H*-imidazole (**3e**) [12]



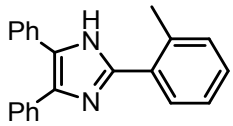

Starting from 1,2-diphenylethanone (0.4 mmol, 78.4 mg) and 4-bromobenzaldehyde (0.2 mmol, 37 mg) to give the product as a white solid, 49 mg, 66% yield, eluent: petroleum ether/ethyl acetate 8/1. $^{1}$H NMR (400 MHz, DMSO-$d_6$): δ 12.78 (br s, 1H), 8.03 (d, $J$ = 8.5 Hz, 2H), 7.68 (d, $J$ = 8.4 Hz, 2H), 7.53-7.51 (m, 4H), 7.35 (br s, 6H); $^{13}$C NMR (125 MHz, DMSO-$d_6$): δ 144.5, 137.3, 134.9, 131.6, 129.7, 129.5, 128.4, 127.3, 127.1, 126.7, 121.4.

4,5-diphenyl-2-(4-nitrophenyl)-1*H*-imidazole (**3f**) [14]



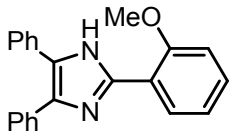

Starting from 1,2-diphenylethanone (0.4 mmol, 78.4 mg) and 4-nitrobenzaldehyde (0.2 mmol, 30.2 mg) to give the product as a yellow solid, 43 mg, 63% yield, eluent: petroleum ether/ethyl acetate 8/1. $^{1}$H NMR (400 MHz, DMSO-$d_6$): δ 13.13 (br s, 1H), 8.36-8.31 (m, 4H), 7.54 (d, $J$ = 7.2 Hz, 4H), 7.39-7.37 (m, 6H); $^{13}$C NMR (125 MHz, DMSO-$d_6$): δ 146.5, 143.4, 136.1, 128.4, 127.1, 125.7, 124.2.

2-(2-methylphenyl)-4,5-diphenyl-1*H*-imidazole (**3g**) [11]



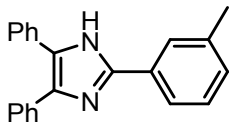
Starting from 1,2-diphenylethanone (0.4 mmol, 78.4 mg) and 2-methylbenzaldehyde (0.2 mmol, 23.2 μL) to give the product as a white solid, 46 mg, 74% yield, eluent: petroleum ether/ethyl acetate 8/1. $^{1}$H NMR (400 MHz, DMSO-$d_6$): δ 12.63 (br s, 1H), 7.93 (s, 1H), 7.87 (d, $J$ = 7.7 Hz, 1H), 7.52-7.18 (m, 12H), 2.38 (s, 3H); $^{13}$C NMR (125 MHz, DMSO-$d_6$): δ 145.6, 137.8, 130.2, 128.9, 128.5, 128.3, 125.7, 125.1, 122.3, 21.1.

2-(2-methoxyphenyl)-4,5-diphenyl-1*H*-imidazole (**3h**) [11]



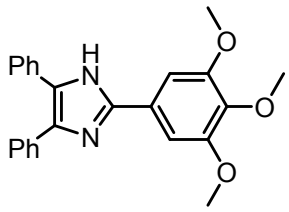
Starting from 1,2-diphenylethanone (0.4 mmol, 78.4 mg) and 2-methoxylbenzaldehyde (0.2 mmol, 28 mg) to give the product as a white solid, 45 mg, 69% yield, eluent: petroleum ether/ethyl acetate 4/1.$^{1}$H NMR (400 MHz, DMSO-$d_6$): δ 11.88 (br s, 1H), 8.05 (dd, $J$ = 7.6, 1.1 Hz, 1H), 7.53 (d, $J$ = 7.6 Hz, 2H), 7.47 (d, $J$ = 7.3 Hz, 2H), 7.44-7.35 (m, 4H), 7.31-7.27 (m, 2H), 7.23-7.15 (m, 2H), 7.09-7.05 (m, 1H); $^{13}$C NMR (125 MHz, DMSO-$d_6$): δ 160.0, 143.1, 136.4, 135.2, 131.2, 129.7, 128.8, 128.6, 128.5, 128.1, 127.6, 127.4, 127.1, 126.4, 120.6, 118.9, 111.6, 55.5.

2-(3-methylphenyl)-4,5-diphenyl-1*H*-imidazole (**3i**) [11]



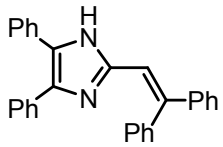
Starting from 1,2-diphenylethanone (0.4 mmol, 78.4 mg) and 3-methylbenzaldehyde (0.2 mmol, 24 μL) to give the product as a white solid, 50 mg, 81% yield, eluent: petroleum ether/ethyl acetate 8/1. $^{1}$H NMR (400 MHz, DMSO-$d_6$): δ 12.63 (br s, 1H), 7.93 (s, 1H), 7.88 (d, $J$ = 7.8 Hz, 1H), 7.55 (d, $J$ = 7.6 Hz,2H), 7.50 (d, $J$ = 7.6 Hz, 2H), 7.46-7.42 (m, 2H), 7.39-7.28 (m, 4H), 7.24-7.18 (m, 2H), 2.39 (s, 3H); $^{13}$C NMR (125 MHz, DMSO-$d_6$): δ 145.6, 137.8, 137.0, 135.2, 131.0, 130.2, 128.9, 128.6, 128.5, 128.4, 128.1, 128.1, 127.7, 127.0, 126.4, 125.7, 122.3, 21.0.

2-(3,4,5-trimethoxyphenyl)-4,5-diphenyl-1*H*-imidazole (**3j**) [14]



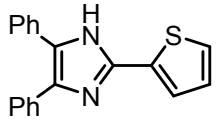
Starting from 1,2-diphenylethanone (0.4 mmol, 78.4 mg) and 3,4,5-trimethoxybenzaldehyde (0.2 mmol, 39 mg) to give the product as a white solid, 56 mg, 73% yield, eluent: petroleum ether/ethyl acetate 4/1. $^{1}$H NMR (400 MHz, DMSO-d$_6$): δ 12.60 (br s, 1H), 7.55 (d, *J* = 7.2 Hz, 2H), 7.50-7.41 (m, 7H), 7.32-7.28 (m, 2H), 7.24-7.20 (m, 1H); $^{13}$C NMR (125 MHz, DMSO-*d*$_6$): δ 153.1, 145.4, 137.7, 136.9, 135.1, 131.2, 128.7, 128.5, 128.2, 128.1, 127.8, 127.0, 126.5, 125.8, 102.6, 60.1, 56.0.

2-(2,2-diphenylvinyl)-4,5-diphenyl-1*H*-imidazole (**3k**)



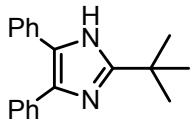
Starting from 1,2-diphenylethanone (0.4 mmol, 78.4 mg) and 3,3-diphenylacrylaldehyde (0.2 mmol, 42 mg) to give the product as a white solid, 38 mg, 48% yield, eluent: petroleum ether/ethyl acetate 8/1. $^{1}$H NMR (400 MHz, DMSO-*d*$_6$): δ 11.81 (br s, 1H), 7.44-7.37 (m, 7H), 7.33-7.28 (m, 10H), 7.21-7.12 (m, 3H), 6.90 (s, 1H); $^{13}$C NMR (125 MHz, DMSO-*d*$_6$): δ 144.0, 142.9, 142.1, 139.5, 136.9, 135.1, 131.0, 130.1, 128.7, 128.5, 128.0, 127.9, 127.9, 127.7, 127.6, 127.4, 127.2, 126.8, 126.8, 126.4, 115.6; FT-IR (film): 3411, 3065, 3027, 1599, 1577, 1508, 1496, 1449, 1441, 1235, 1027, 967, 764, 692, 591 cm$^{-1}$; HRMS (ESI) calcd for $C_{29}H_{22}N_2$ $[M+H]^+$ 399.1856, found 399.1858; mp: 191-193 $^{o}$C.

4,5-diphenyl-2-(thiophen-2-yl)-1*H*-imidazole (**3l**) [10]



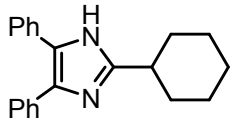
Starting from 1,2-diphenylethanone (0.4 mmol, 78.4 mg) and thiophene-2-carbaldehyde (0.2 mmol, 18.5 μL) to give the product as a yellow solid, 35 mg, 58% yield, eluent: petroleum ether/ethyl acetate 8/1. $^{1}$H NMR (400 MHz, DMSO-*d*$_6$): δ 12.80 (br s, 1H), 7.68 (d, *J* = 3.2 Hz, 1H), 7.54 (d, *J* = 4.8 Hz, 1H), 7.48-7.24 (m, 10H); 7.15-7.13 (m, 1H); $^{13}$C NMR (125 MHz, DMSO-*d*$_6$): δ 141.7, 136.9, 134.9, 133.9, 130.9, 128.8, 128.3, 128.0, 127.2, 126.7, 126.4, 124.4.

2-(*tert*-butyl)-4,5-diphenyl-1*H*-imidazole (**3m**) [15]



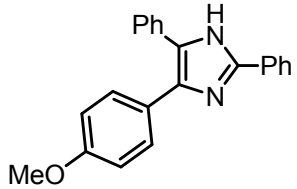
Starting from 1,2-diphenylethanone (0.4 mmol, 78.4 mg) and pivalaldehyde (0.2 mmol, 22 μL) to give the product as a white solid, 19 mg, 34% yield, eluent: petroleum ether/ethyl acetate 4/1. $^{1}$H NMR (400 MHz, DMSO-$d_6$): δ 11.80 (br s 1H), 7.46 (d, $J$ = 7.6 Hz, 2H), 7.40-7.37 (m, 4H), 7.33-7.31 (m, 1H), 7.24 (t, $J$ =7.6 Hz, 2H), 7.15 (t, $J$ = 7.2 Hz, 1H), 1.37 (s, 9H); $^{13}$C NMR (125 MHz, DMSO-$d_6$): δ 155.4, 135.7, 134.4, 131.6, 128.6, 128.4, 128.3, 128.1, 128.0, 127.2, 126.9, 126.4, 125.9, 32.6, 29.4.

2-cyclohexyl-4,5-diphenyl-1*H*-imidazole (**3n**) [13]



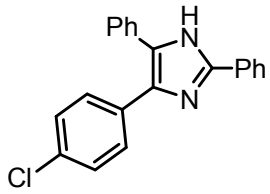
Starting from 1,2-diphenylethanone (0.4 mmol, 78.4 mg) and cyclohexanecarbaldehyde (0.2 mmol, 24.2 μL) to give the product as a white solid, 12 mg, 20% yield, eluent: petroleum ether/ethyl acetate 4/1. $^{1}$H NMR (400 MHz, DMSO-$d_6$): δ 11.90 (br s, 1H), 7.45-7.18 (m, 10H), 2.73-2.67 (m, 1H), 1.99-1.95 (m, 2H), 1.83-1.78 (m, 2H), 1.70-1.68 (m, 1H), 1.63-1.54 (m, 2H), 1.40-1.29 (m, 3H); $^{13}$C NMR (125 MHz, DMSO-$d_6$): δ 152.9, 136.3, 129.0, 128.5, 128.3, 127.5, 126.5, 37.7, 32.0, 26.2, 26.1.

4-(4-methoxyphenyl)-2,5-diphenyl-1*H*-imidazole (**3o**) [16]



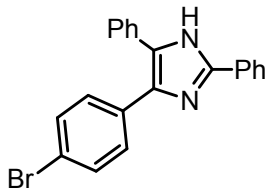
Starting from 2-(4-methoxyphenyl)-1-phenylethanone(0.4 mmol, 90 mg) and benzaldehyde (0.2 mmol, 20.4 μL) to give the product as a white solid, 46 mg, 70% yield; Starting from 1-(4-methoxyphenyl)-2-phenylethanone (0.4 mmol, 90 mg) and benzaldehyde (0.2 mmol, 20.4 uL) to give the product as a white solid, 41 mg, 63% yield; eluent: petroleum ether/ethyl acetate 4/1. $^{1}$H NMR (400 MHz, DMSO-$d_6$): δ 12.60 (br s, 1H), 8.08 (d, $J$ = 7.8 Hz, 2H), 7.57 (d, $J$ = 7.4 Hz, 1H), 7.52-7.18 (m, 9H), 7.03-6.87 (m, 2H), 3.8 (s, 3H); $^{13}$C NMR (125 MHz, DMSO-$d_6$): δ 158.9, 158.0, 145.2, 145.0, 137.1, 136.4, 135.3, 131.2, 130.4, 130.4, 129.8, 128.6, 128.5, 128.3, 128.2, 128.1, 128.0, 128.0, 127.7, 127.5, 127.2, 126.8, 126.2, 125.1, 125.0, 123.3, 114.1, 113.6, 55.1, 55.0.

4-(4-chlorophenyl)-2,5-diphenyl-1H-imidazole (**3p**) [17]



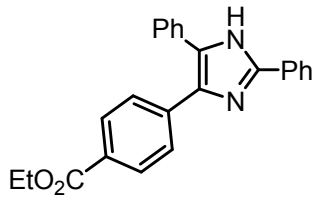

Starting from 1-(4-chlorophenyl)-2-phenylethanone(0.4 mmol, 92.2 mg) and benzaldehyde (0.2 mmol, 20.4 μL) to give the product as a white solid, 43 mg, 65% yield, eluent: petroleum ether/ethyl acetate 8/1. $^1$H NMR (500 MHz, DMSO-$d_6$): δ 12.76 (br s, 1H), 8.07 (d, $J$ = 7.5 Hz, 2H), 7.56-7.47 (m, 8H), 7.42-7.32 (m, 4H); $^{13}$C NMR (125 MHz, DMSO-$d_6$): δ 146.1, 130.5, 129.3, 129.2, 129.0, 128.8, 128.8, 128.7, 128.5, 127.7, 125.7.

4-(4-bromophenyl)-2,5-diphenyl-1*H*-imidazole (**3q**) [17]




Starting from 1-(4-bromophenyl)-2-phenylethanone(0.4 mmol, 110 mg) and benzaldehyde (0.2 mmol, 20.4 μL) to give the product as a white solid, 59 mg, 79% yield, eluent: petroleum ether/ethyl acetate 8/1. $^1$H NMR (400 MHz, DMSO-$d_6$): δ 12.76 (br s, 1H), 8.08 (d, $J$ = 7.4 Hz, 2H), 7.61-7.27 (m, 12H); $^{13}$C NMR (125 MHz, DMSO-$d_6$): δ 145.7, 137.7, 135.8, 134.9, 134.4, 131.6, 131.1, 130.8, 130.2, 128.9, 128.8, 128.7, 128.5, 128.4, 128.3, 128.0, 127.3, 127.0, 126.8, 125.2, 120.7, 119.5.

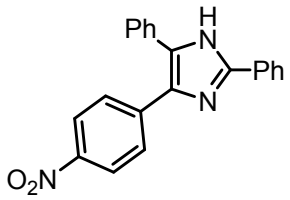
2,5-diphenyl-4-(4-ethoxylcarbonylphenyl)-1*H*-imidazole (**3r**)




Starting from ethyl 4-(2-oxo-2-phenylethyl)benzoate (0.4 mmol, 107 mg) and benzaldehyde (0.2 mmol, 20.4 μL) to give the product as a white solid, 66 mg, 90% yield, eluent: petroleum ether/ethyl acetate 4/1. $^1$H NMR (500 MHz, DMSO-$d_6$): δ 12.85 (br s, 12.85), 8.08 (d, $J$ = 7.4 Hz, 2H), 7.96-7.87 (m, 2H), 7.68-7.67 (m, 2H), 7.52-7.28 (m, 8H), 4.30 (q, $J$ = 6.8 Hz, 2H), 1.31 (t, $J$ = 6.8 Hz, 3H); $^{13}$C NMR (125 MHz, DMSO-$d_6$): δ 165.5, 146.4, 145.9, 139.8, 135.7, 130.7, 130.0, 129.9, 129.4, 129.1, 128.8, 128.7, 128.5, 128.4, 128.3, 128.2, 128.0, 127.5, 126.9, 126.6, 125.4, 125.2, 60.7, 60.5, 14.1; FT-IR (film): 3429, 3283, 3061, 2979, 1712, 1676, 1608, 1487, 1460, 1282,

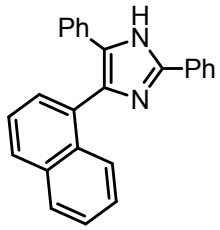
1108, 1020, 769, 698 $cm^{-1}$; HRMS (ESI) calcd for $C_{24}H_{20}N_2O_2$ $[M+H]^+$ 369.1598, found 369.1596; mp: 198-200 °C.

4-(4-nitrophenyl)-2,5-diphenyl-1*H*-imidazole (**3s**)



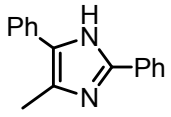
Starting from 2-(4-nitrophenyl)-1-phenylethanone (0.4 mmol, 96.4 mg) and benzaldehyde (0.2 mmol, 20.4 μL) to give the product as a yellow solid, 31 mg, 45% yield, eluent: petroleum ether/ethyl acetate 4/1. $^1$H NMR (500 MHz, DMSO-$d_6$): δ 12.99 (br s, 1H), 8.18 (d, $J$ = 7.6 Hz, 2H), 8.09 (d, $J$ = 7.5 Hz, 2H), 7.78 (d, $J$ = 8.4 Hz, 2H), 7.54-7.40 (m, 8H); $^{13}$C NMR (125 MHz, DMSO-$d_6$): δ 146.6, 145.6, 129.9, 129.0, 128.9, 128.8, 127.4, 125.5, 123.8; FT-IR (film): 3342, 3061, 2919, 1595, 1508, 1485, 1327, 1107, 856, 773, 719, 691 $cm^{-1}$; HRMS (ESI) calcd for $C_{21}H_{15}N_3O_2$ $[M+H]^+$ 342.1237, found 342.1238; mp: 233-235 °C.

4-(naphthalen-1-yl)-2,5-diphenyl-1*H*-imidazole (**3t**)



Starting from 2-(naphthalen-1-yl)-1-phenylethanone (0.4 mmol, 98 mg) and benzaldehyde (0.2 mmol, 20.4 μL) to give the product as a white solid, 57 mg, 82% yield, eluent: petroleum ether/ethyl acetate 8/1. $^1$H NMR (500 MHz, DMSO-$d_6$): δ 12.91 (br s, 1H), 8.12-7.02 (m, 17H); $^{13}$C NMR (125 MHz, DMSO-$d_6$): δ 145.9, 145.6, 138.0, 137.1, 134.8, 133.6, 133.5, 133.4, 132.0, 130.4, 129.5, 129.4, 129.1, 129.0, 128.8, 128.8, 128.5, 128.4, 128.2, 128.1, 127.9, 127.0, 126.9, 126.7, 126.4, 126.2, 126.1, 126.1, 126.0, 125.9, 125.8, 125.8, 125.6, 125.5, 125.1; FT-IR (film): 3417, 3054, 1604, 1588, 1490, 1461, 1400, 1383, 802, 777, 695 $cm^{-1}$; HRMS (ESI) calcd for $C_{25}H_{18}N_2$ $[M+H]^+$ 347.1543, Found 347.1545; mp: 263-265 °C.

4-methyl-2,5-diphenyl-1*H*-imidazole (**3u**) [18]



Starting from propiophenone (0.4 mmol, 53.6 mg) and benzaldehyde (0.2 mmol, 20.4 μL) to give the product as a white solid, 19 mg, 40% yield, eluent: petroleum ether/ethyl acetate 4/1. $^{1}$H NMR (400 MHz, DMSO-$d_6$): δ 12.38 (br s, 1H), 8.00-7.94 (m, 2H), 7.73-7.59 (m, 2H), 7.51-7.20 (m, 6H), 2.48 (s, 3H); $^{13}$C NMR (125 MHz, DMSO-$d_6$): δ 143.5, 136.3, 135.5, 130.6, 128.7, 128.3, 127.7, 126.5, 125.9, 125.6, 125.0, 124.5, 124.2, 29.0, 11.3.

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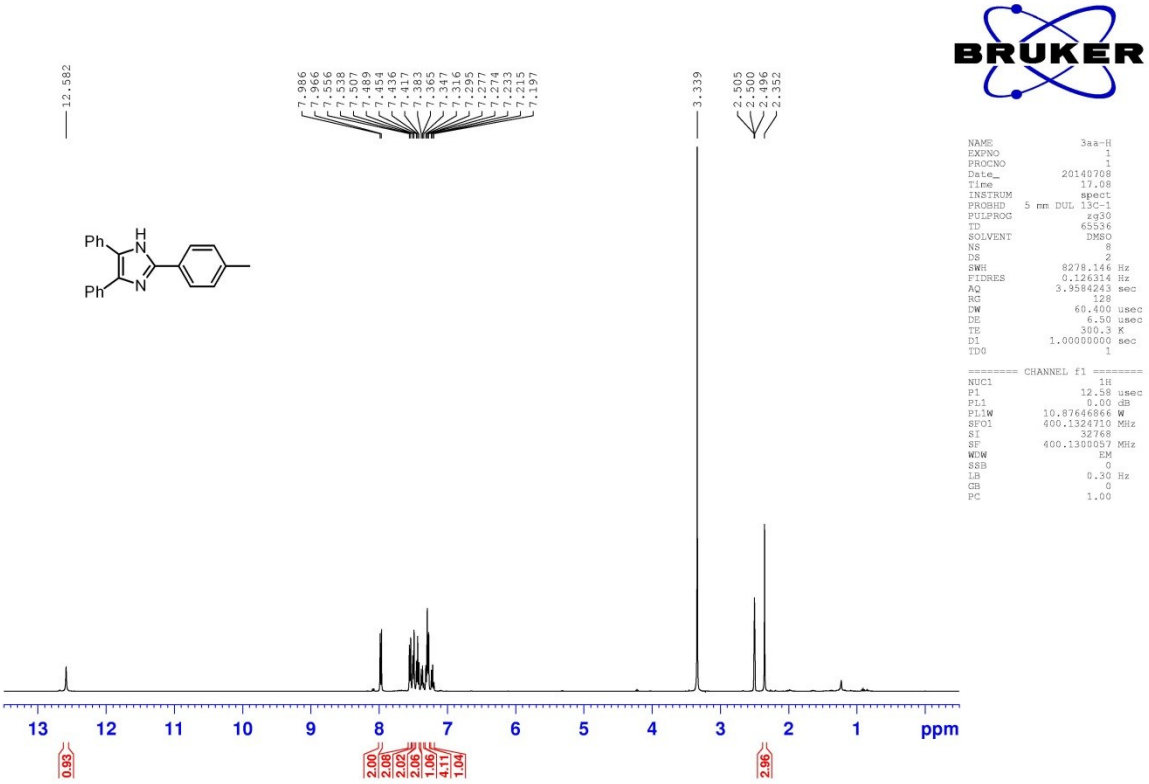
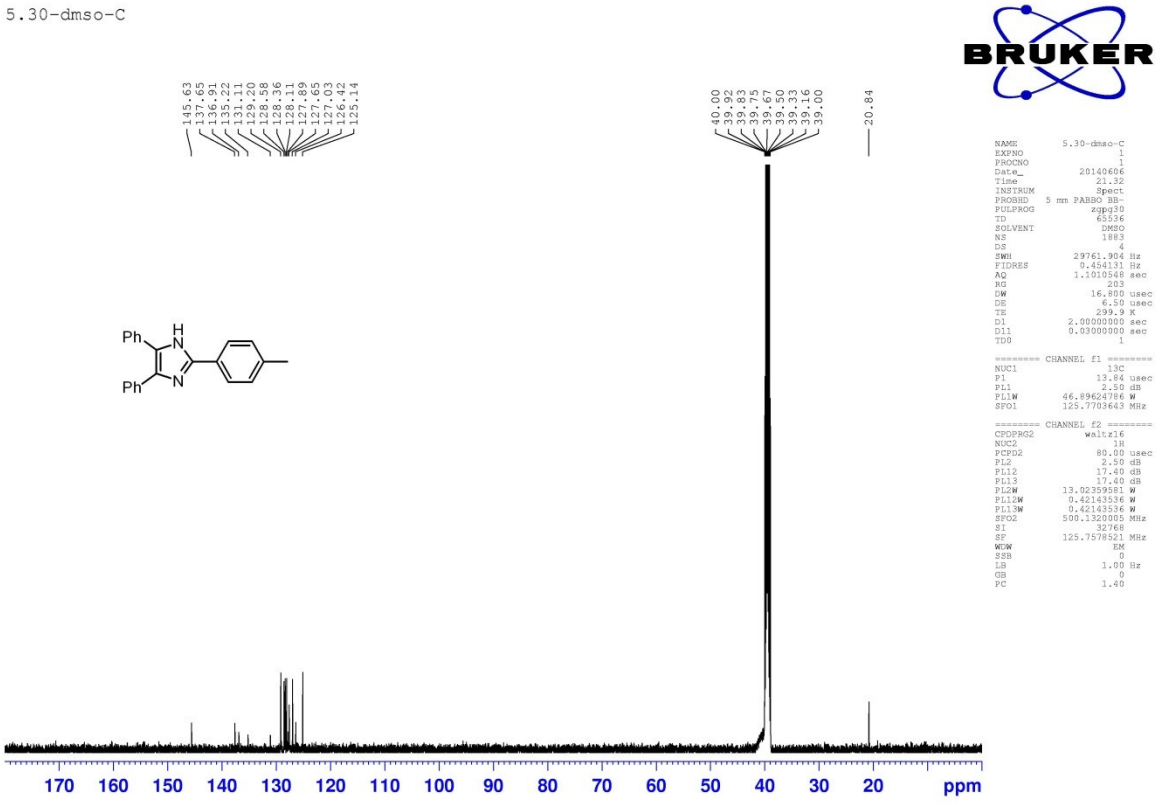
# VI. Copies of $^{1}H$ NMR and $^{13}C$ NMR Spectra

**3a**

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136.91
135.22
131.11
129.60
128.68
128.36
128.11
127.89
127.65
127.03
126.42
125.14
40.00
39.92
39.83
39.75
39.67
39.50
39.33
39.16
39.00
20.84
Ph
Ph
H
N
N
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PROCNO 1
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Time 21.32
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PULPROG zgpg30
TD 65536
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FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 299.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 13.84 usec
PL1 2.50 dB
PL1W 46.89624786 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
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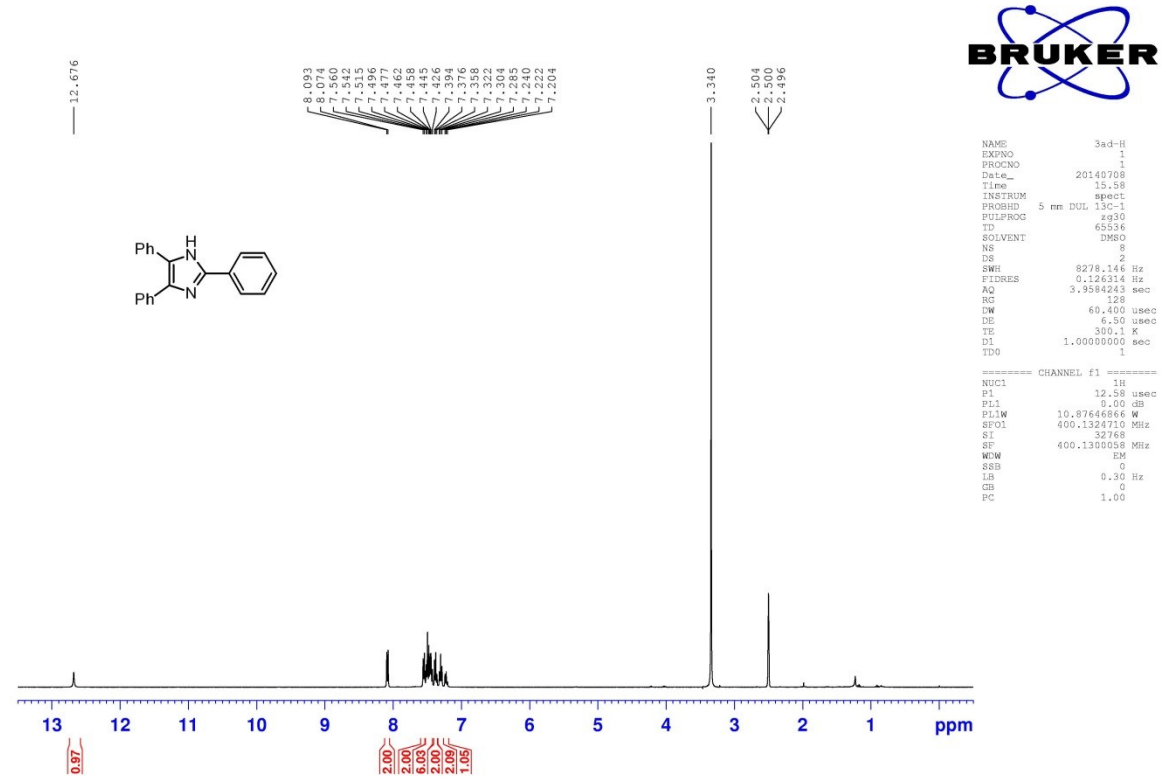
SI 32768
SF 125.7578521 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

**3b**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8.074
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7.496
7.477
7.462
7.458
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7.426
7.394
7.376
7.358
7.322
7.304
7.285
7.240
7.222
7.204
3.340
2.504
2.500
2.496
Ph
Ph
H
N
N
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2.00
2.00
6.03
2.00
2.09
1.05
NAME 3ad-H
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PROCNO 1
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Time 15.58
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PULPROG zg30
TD 65536
SOLVENT DMSO
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DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
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RG 128
DW 60.400 usec
DE 6.50 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1
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NUC1 1H
P1 12.58 usec
PL1 0.00 dB
PL1W 10.87646866 W
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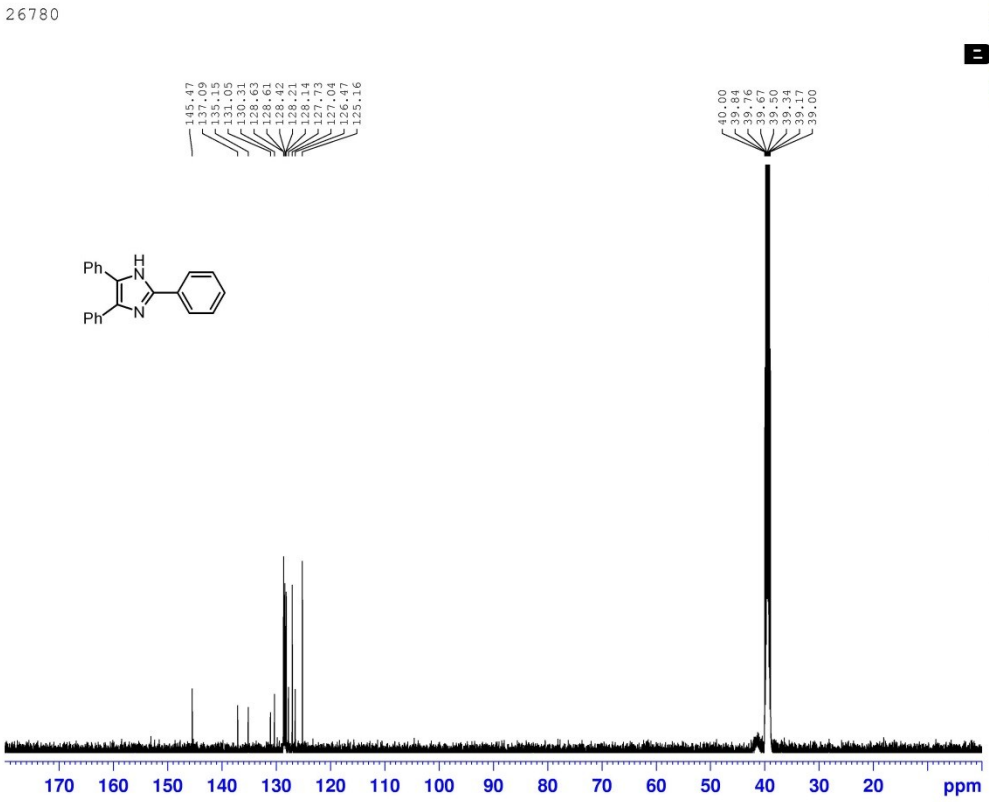
GB 0
PC 1.00





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PULPROG zgpg30
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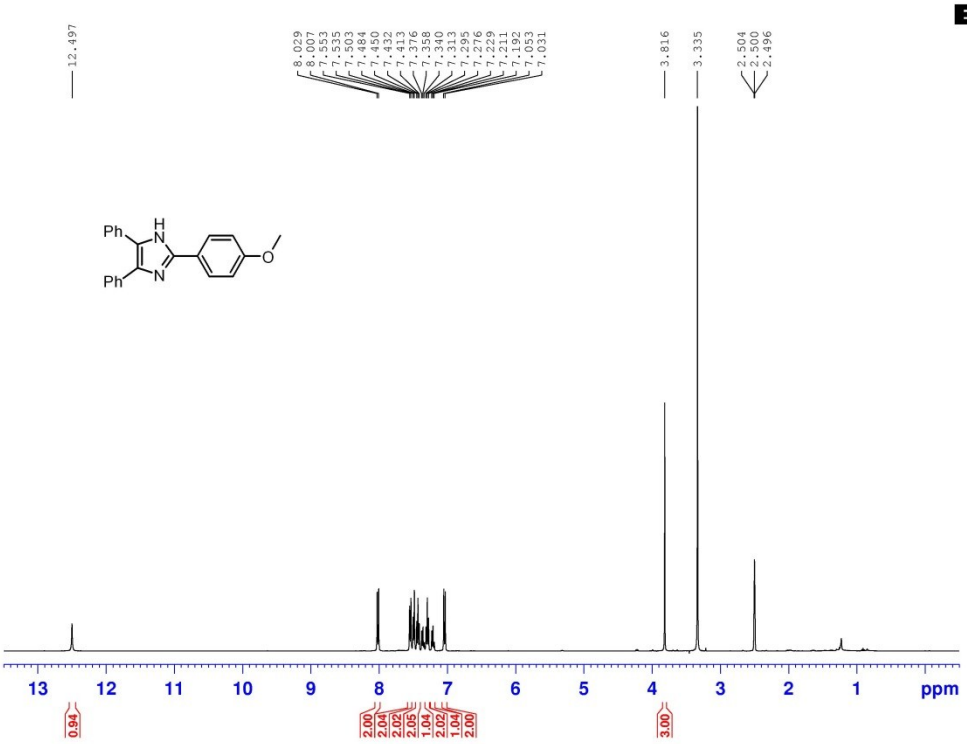
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 13.84 usec
PL1 2.50 dB
PL1W 46.89624786 W
SFO1 125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7578532 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


**3c**





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PROCNO 1
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SWH 8278.146 Hz
FIDRES 0.126314 Hz
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RG 128
DW 60.400 usec
DE 6.50 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1

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PL1 0.00 dB
PL1W 10.87646866 W
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SI 32768
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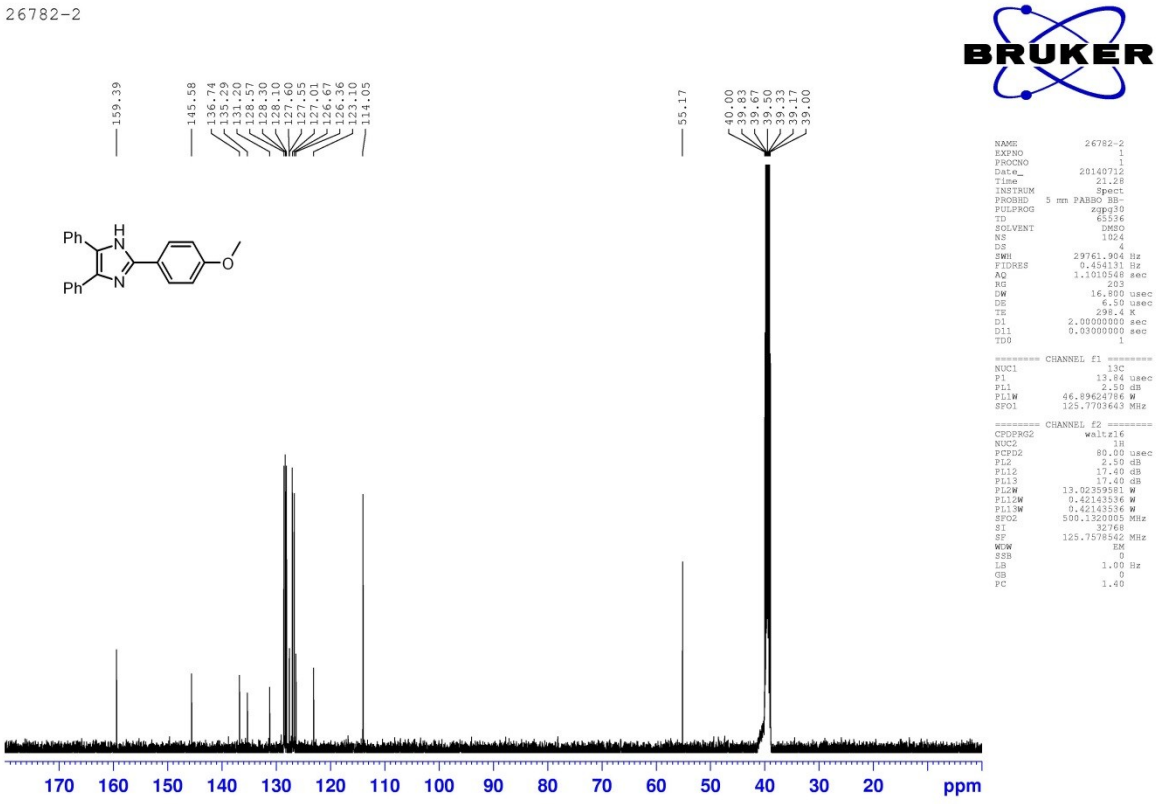
GB 0
PC 1.00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126.36
123.10
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55.17
40.00
39.83
39.67
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39.33
39.17
39.00
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Ph
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O
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FIDRES 0.454131 Hz
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RG 203
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DE 6.50 usec
TE 298.4 K
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D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
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P1 13.84 usec
PL1 2.50 dB
PL1W 46.89624786 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
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SI 32768
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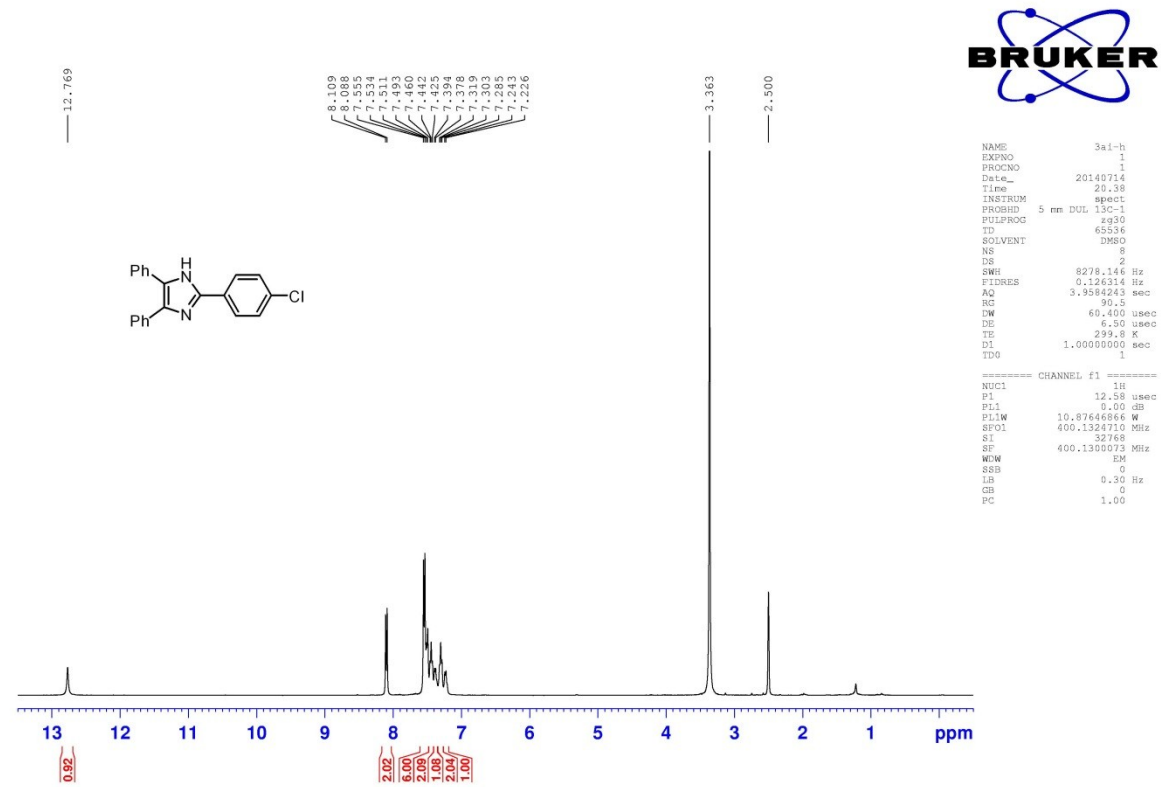
PC 1.40

**3d**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7.511
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7.425
7.394
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7.285
7.243
7.226
3.363
2.500
Ph
H
N
Ph
N
Cl
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6.00
2.09
1.08
2.04
1.00
BRUKER
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PROCNO 1
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RG 90.5
DW 60.400 usec
DE 6.50 usec
TE 299.8 K
D1 1.00000000 sec
TD0 1
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PL1 0.00 dB
PL1W 10.87646866 W
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SI 32768
SF 400.1300073 MHz
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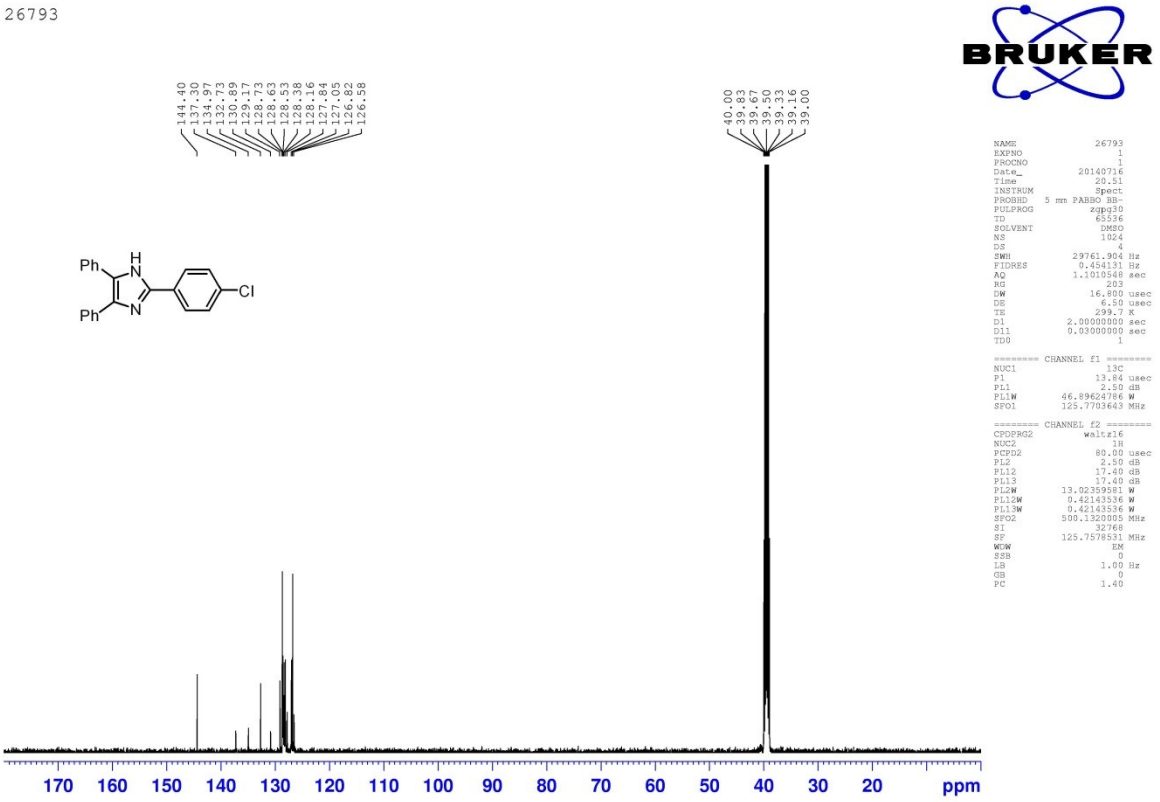
LB 0.30 Hz
GB 0
PC 1.00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128.53
128.38
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126.58
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39.83
39.67
39.50
39.33
39.16
39.00
Ph
H
N
N
Ph
Cl
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PROCNO 1
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DS 4
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FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 299.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 13.84 usec
PL1 2.50 dB
PL1W 46.89624786 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
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SI 32768
SF 125.7578531 MHz
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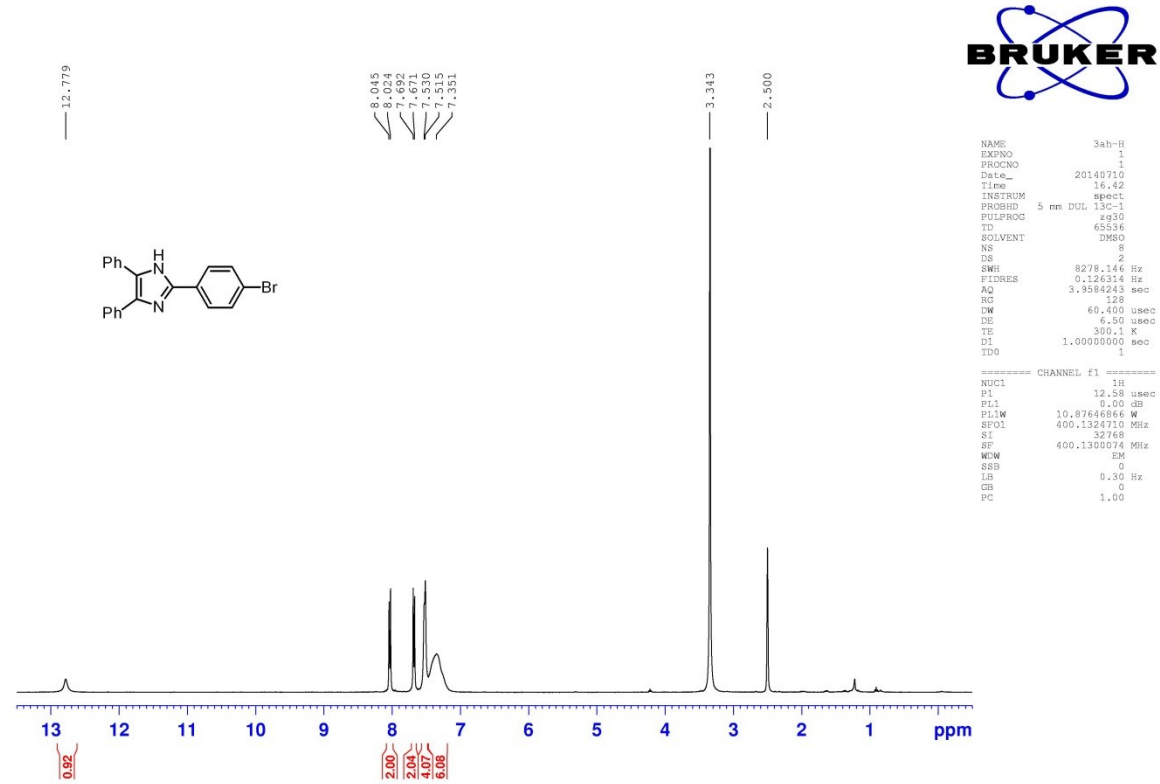
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

**3e**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7.671
7.530
7.515
7.351
3.343
2.500
Ph
H
N
N
Ph
Br
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.92
2.00
2.04
4.07
6.08
NAME 3ah-H
EXPNO 1
PROCNO 1
Date_ 20140710
Time 16.42
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SOLVENT DMSO
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DS 2
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FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 128
DW 60.400 usec
DE 6.50 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.58 usec
PL1 0.00 dB
PL1W 10.87646866 W
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SI 32768
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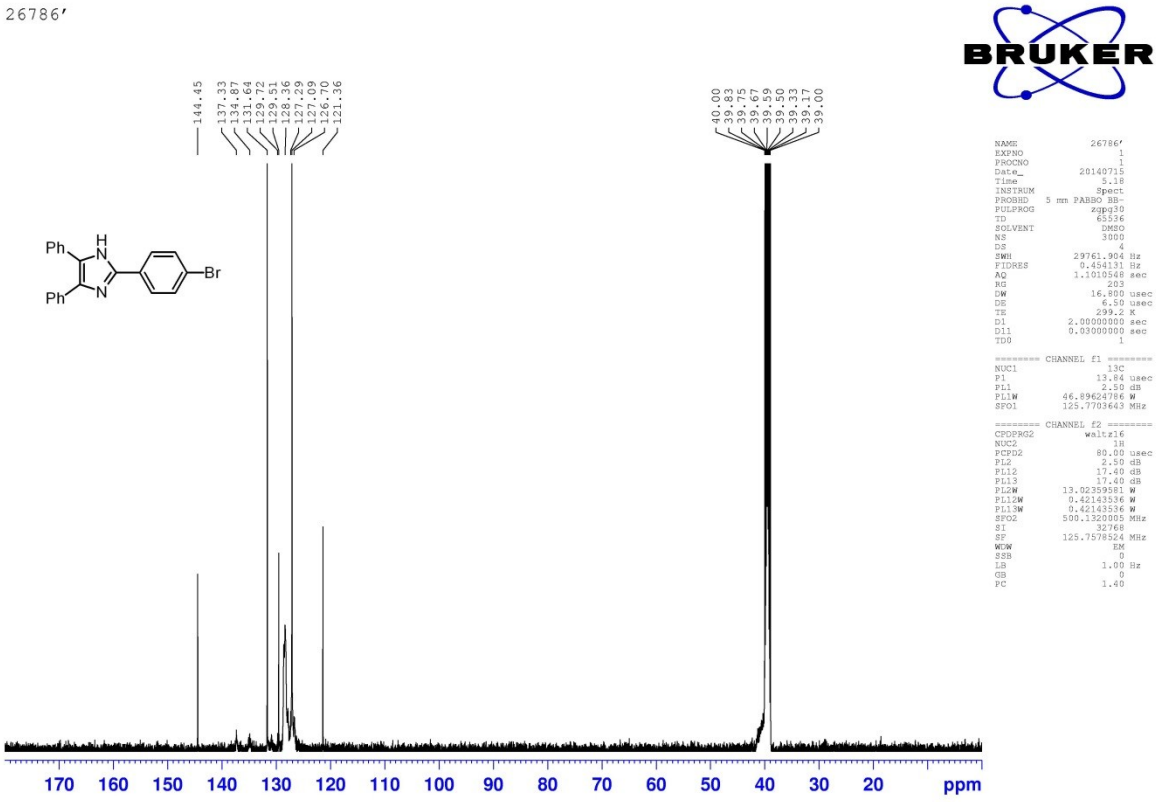
GB 0
PC 1.00





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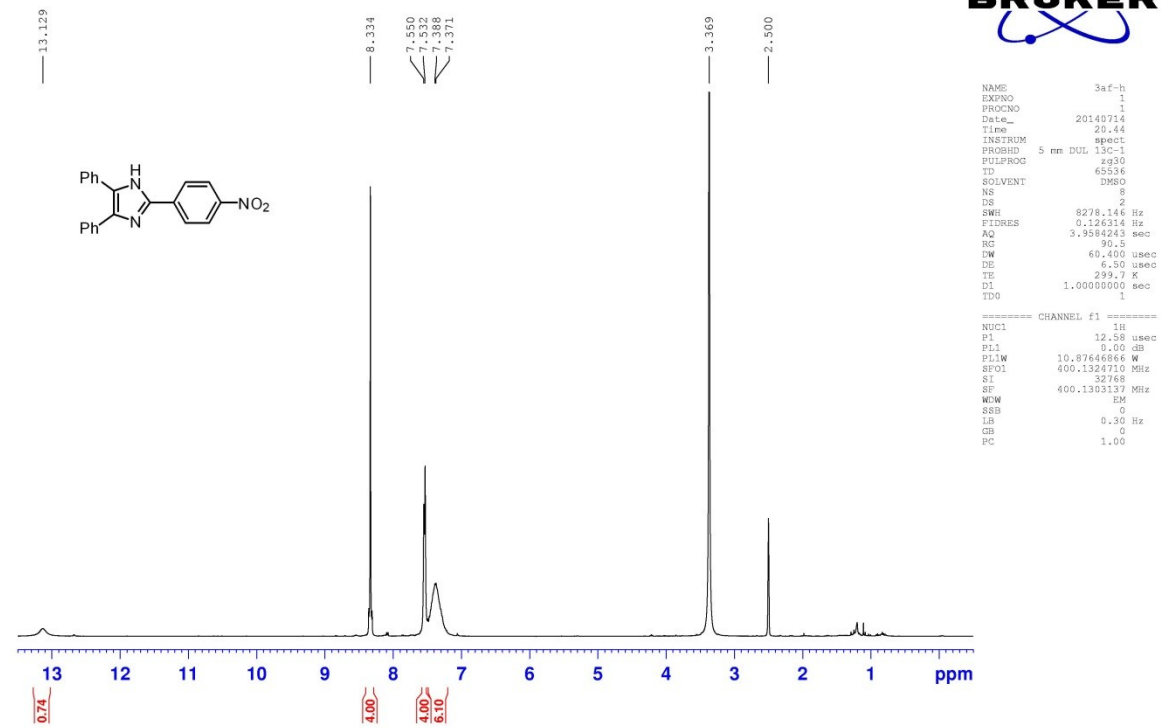
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 13.84 usec
PL1 2.50 dB
PL1W 46.89624786 W
SFO1 125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7578524 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


**3f**





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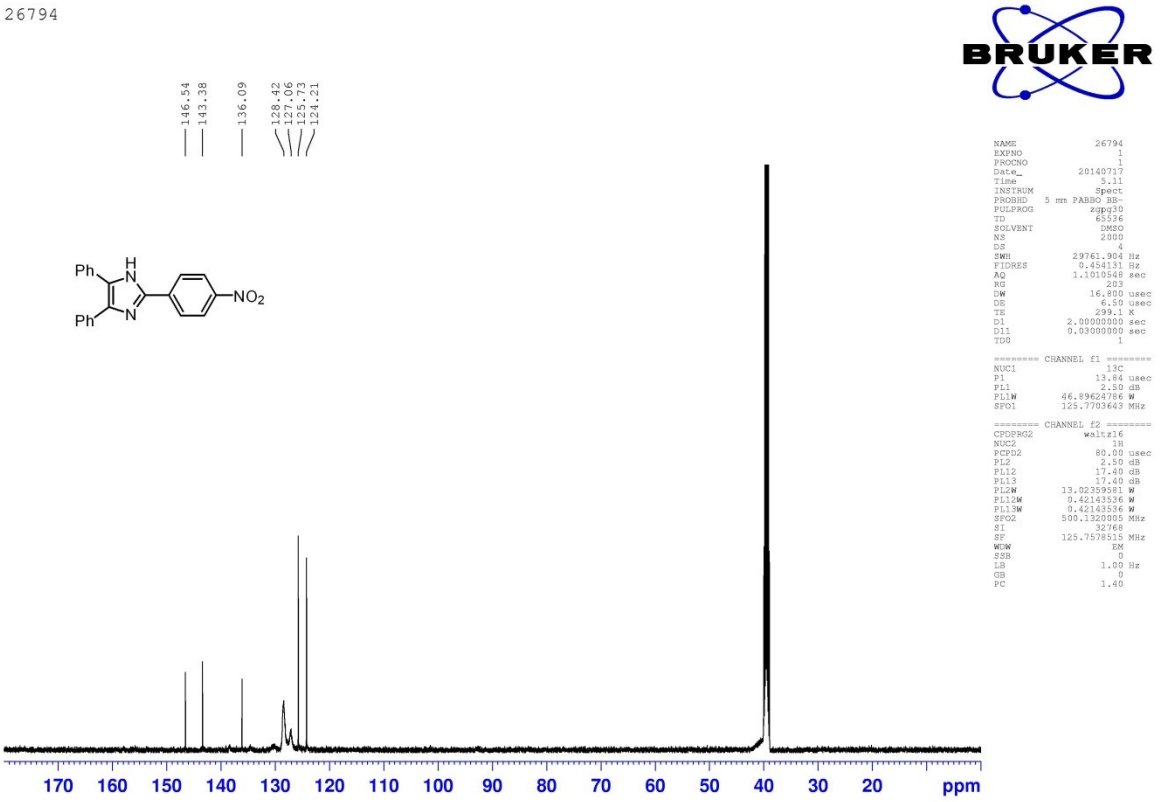
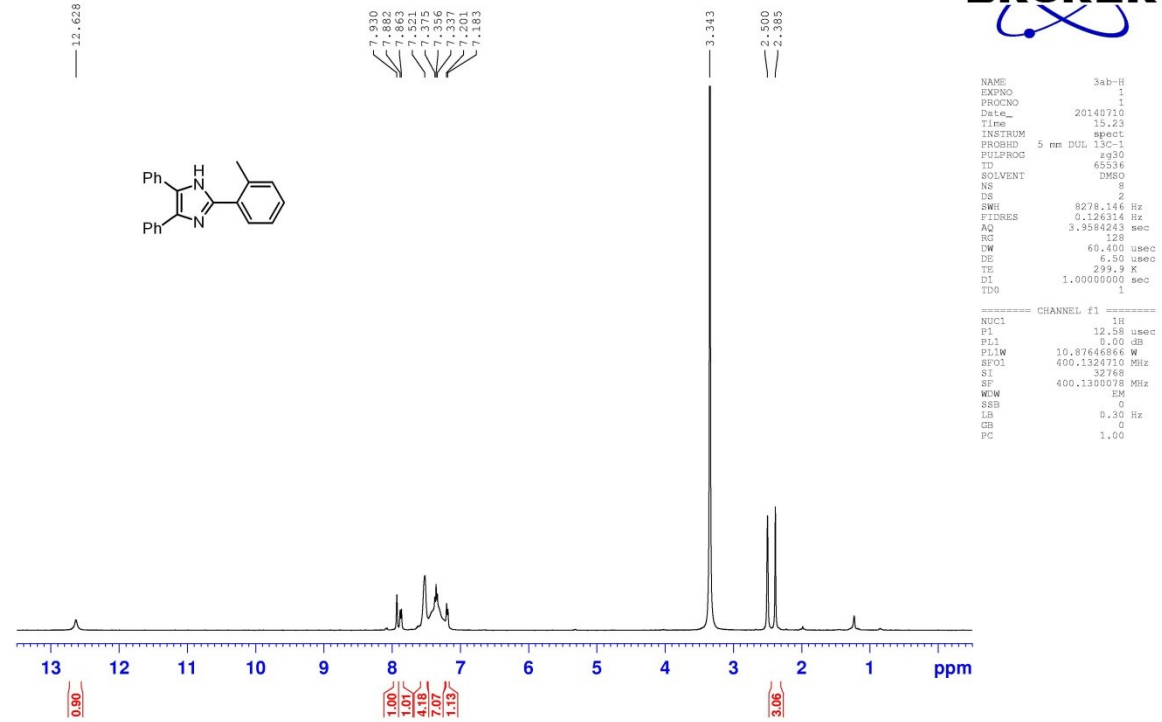
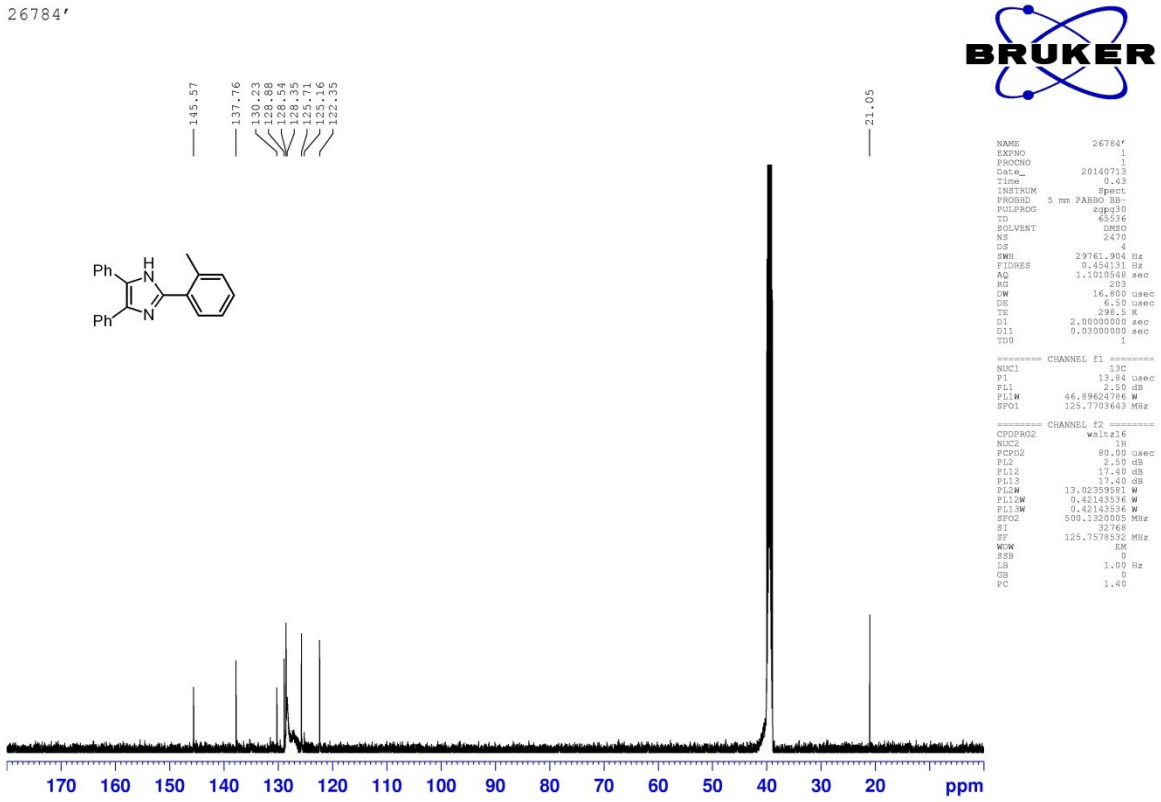
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 90.5
DW 60.400 usec
DE 6.50 usec
TE 299.7 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 12.58 usec
PL1 0.00 dB
PL1W 10.87646866 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1303137 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

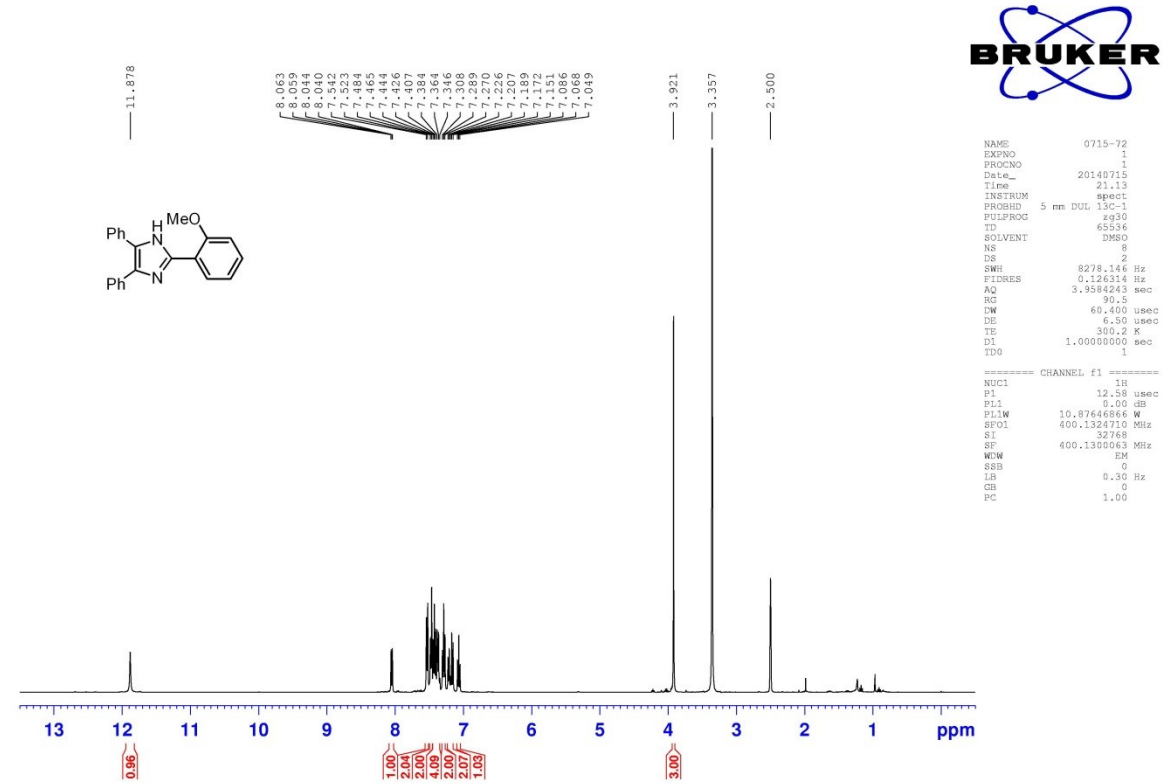

26794
146.54
143.38
136.09
128.42
127.06
125.73
124.21
Ph
Ph
NO2
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

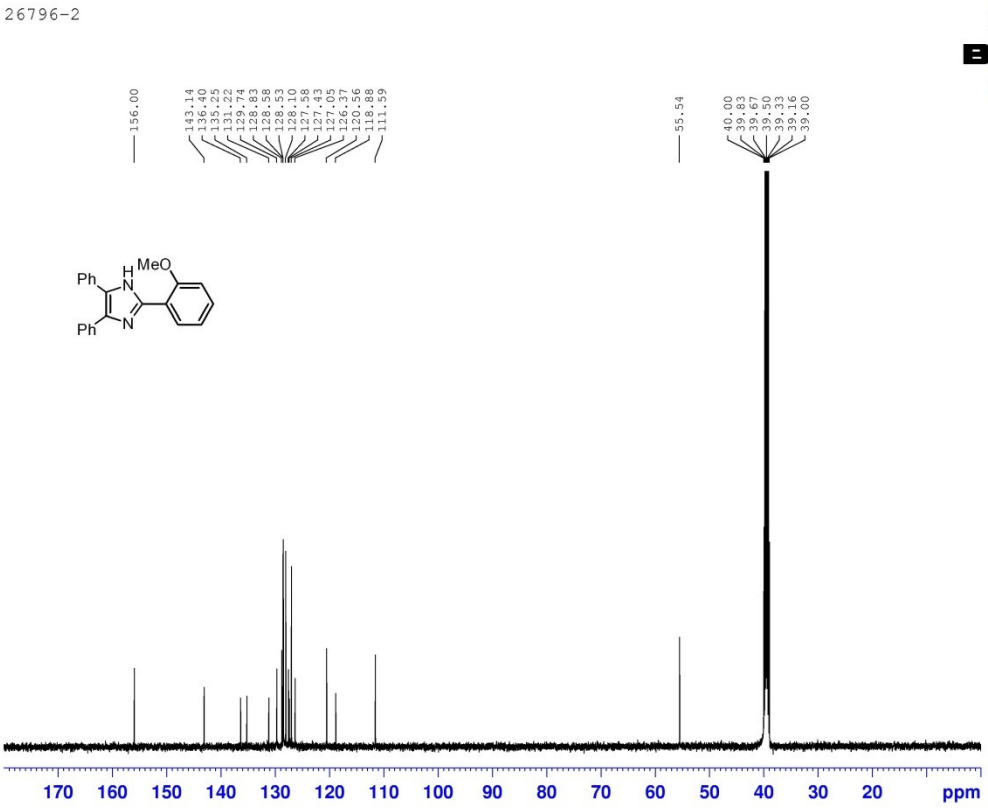
**3g**


12.628
7.930
7.882
7.863
7.521
7.375
7.356
7.337
7.201
7.183
3.343
2.500
2.385
Ph
Ph
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.90
1.00
1.01
4.18
7.07
1.13
3.06


26784′
145.57
137.76
130.23
128.88
128.34
128.35
125.71
125.16
122.35
21.05
Ph
Ph
H
N
N
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm
NAME 26784′
EXPNO 1
PROCNO 1
Date_ 20140713
Time 0.43
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2470
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 13.84 usec
PL1 2.50 dB
PL1W 46.89624786 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7578532 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

**3h**


11.878
8.063
8.059
8.044
8.040
7.542
7.523
7.484
7.465
7.444
7.426
7.407
7.384
7.364
7.346
7.308
7.289
7.270
7.226
7.207
7.189
7.172
7.151
7.086
7.068
7.049
3.921
3.357
2.500
Ph
Ph
H
N
N
MeO
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.96
1.00
2.04
2.00
4.08
2.00
2.07
1.09
3.00
NAME 0715-72
EXPNO 1
PROCNO 1
Date_ 20140715
Time 21.13
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 90.5
DW 60.400 usec
DE 6.50 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.58 usec
PL1 0.00 dB
PL1W 10.87646866 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300063 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



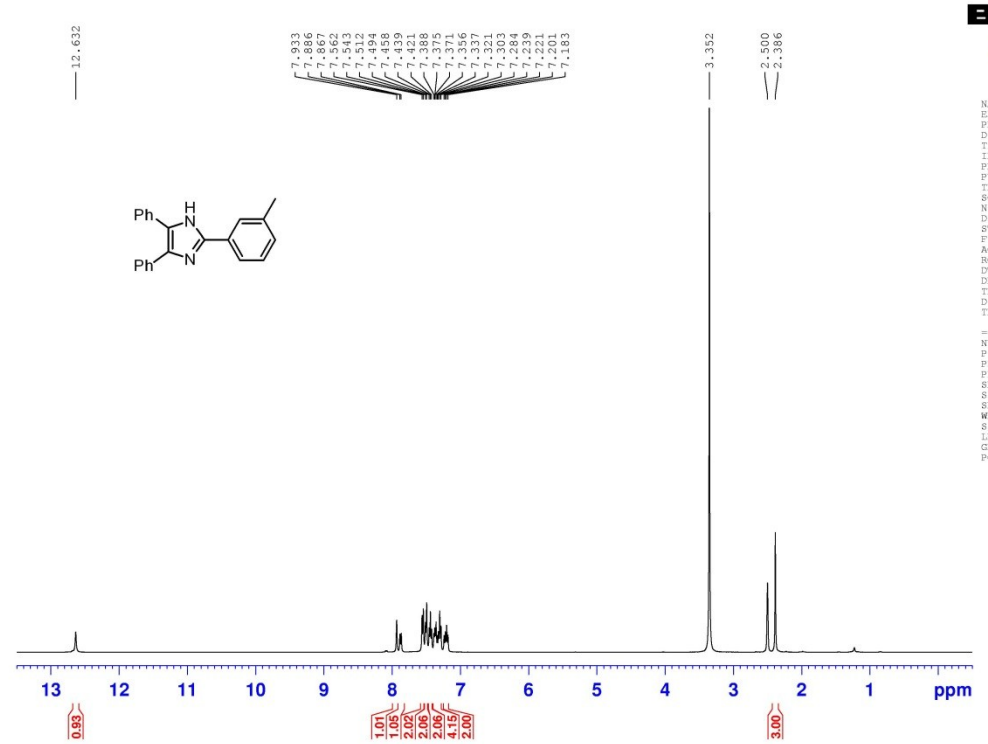


NAME 26796-2
EXPNO 1
PROCNO 1
Date_ 20140717
Time 16.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 13.84 usec
PL1 2.50 dB
PL1W 46.89624786 W
SFO1 125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7578521 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

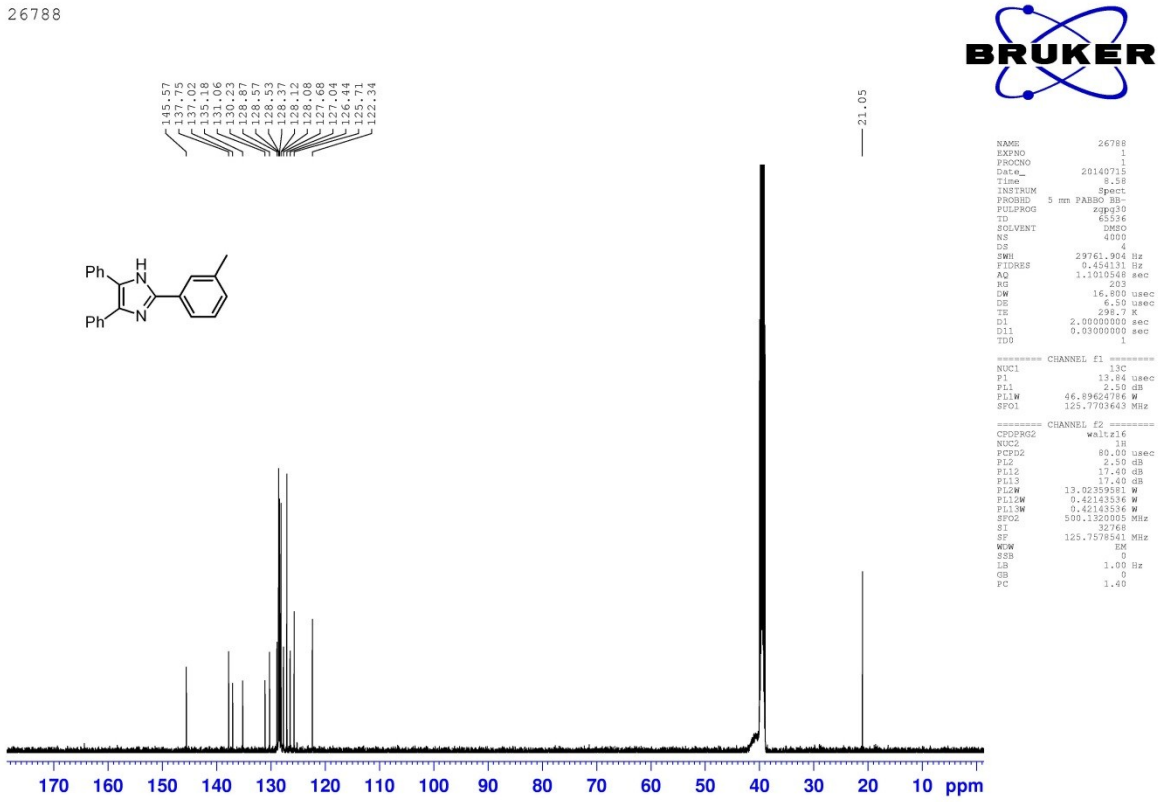

**3i**



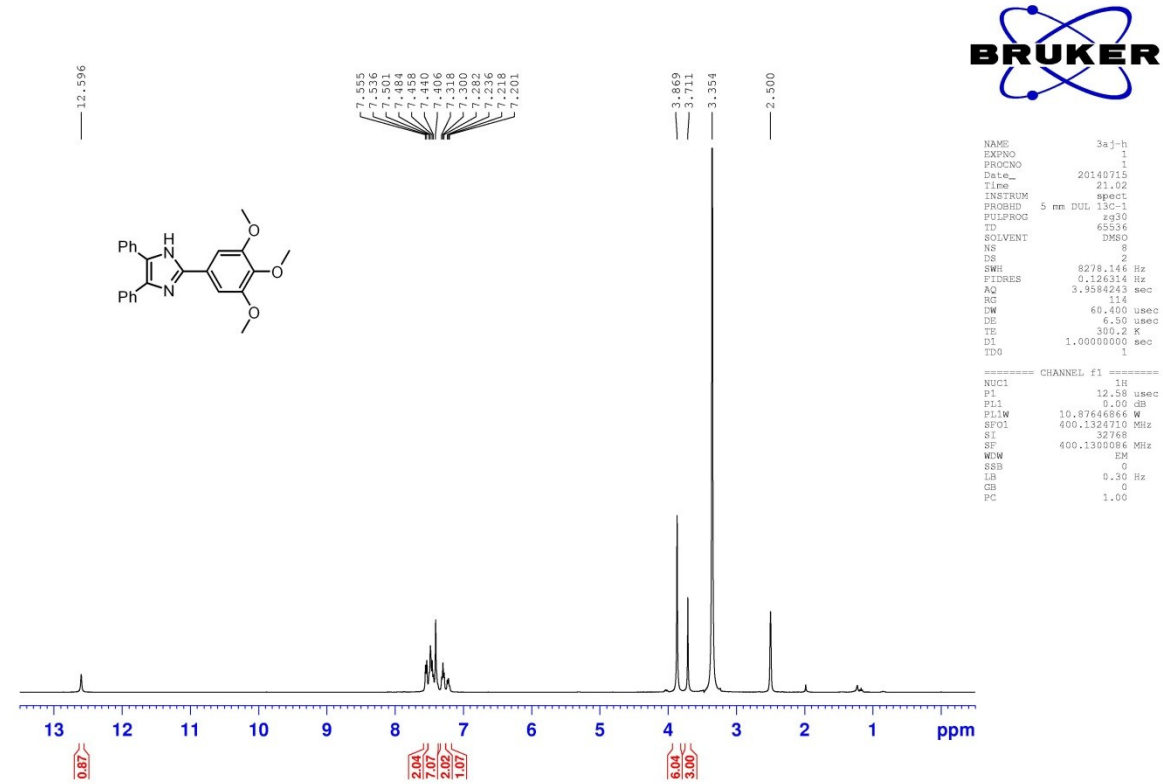


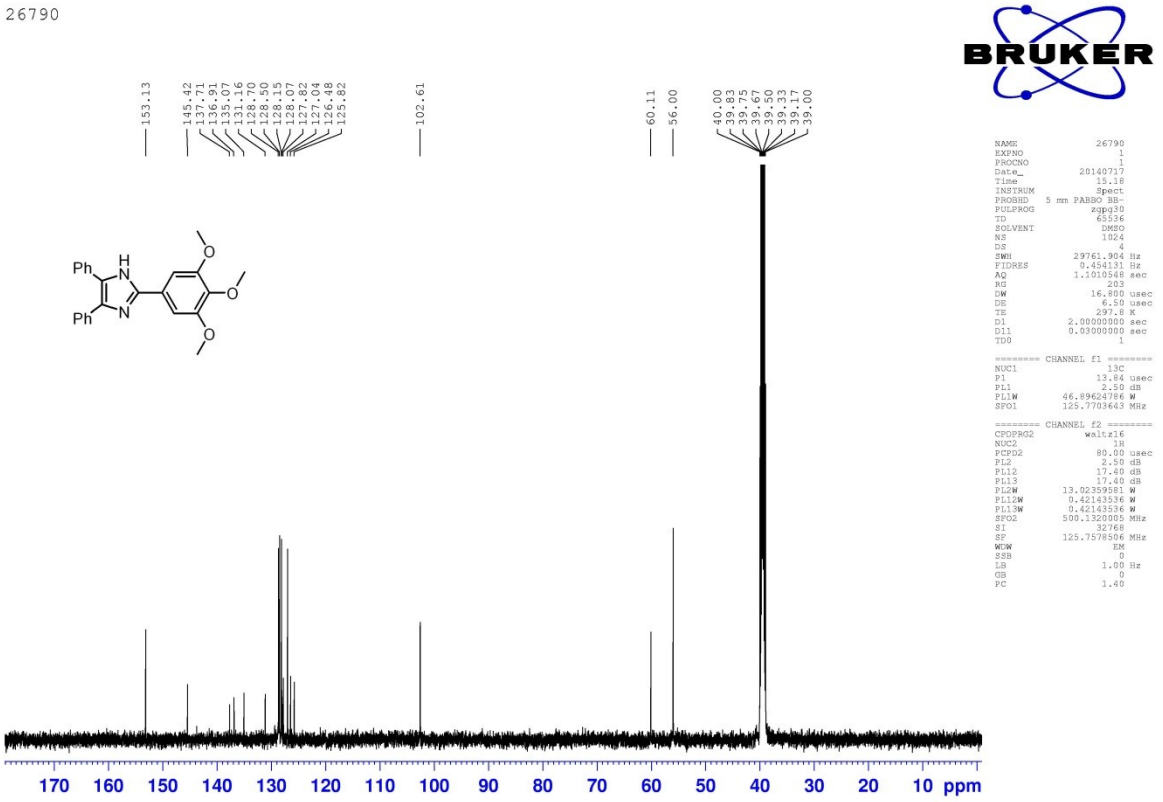
NAME 3ac-H
EXPNO 1
PROCNO 1
Date_ 20140711
Time 15.01
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 128
DW 60.400 usec
DE 6.50 usec
TE 299.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 12.58 usec
PL1 0.00 dB
PL1W 10.87646866 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300074 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

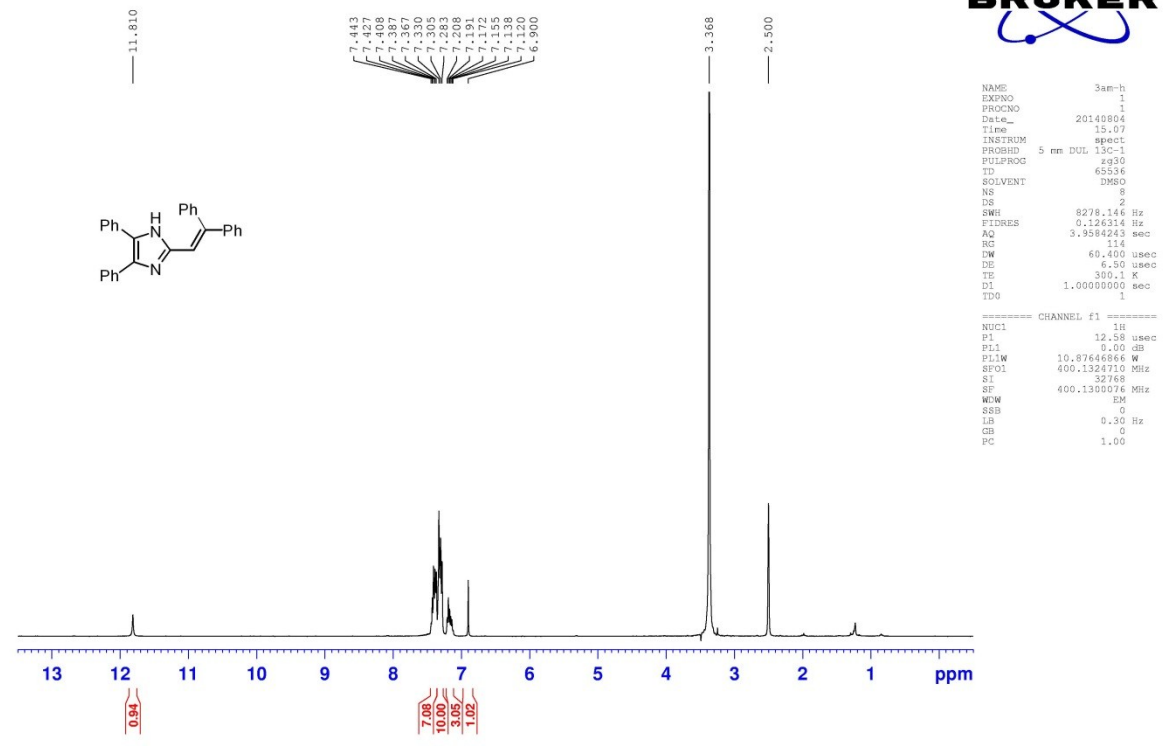

26788
145.57
137.75
137.02
135.18
131.06
130.23
128.87
128.57
128.53
128.37
128.22
128.08
127.68
127.04
126.44
125.71
122.34
21.05
Ph
Ph
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

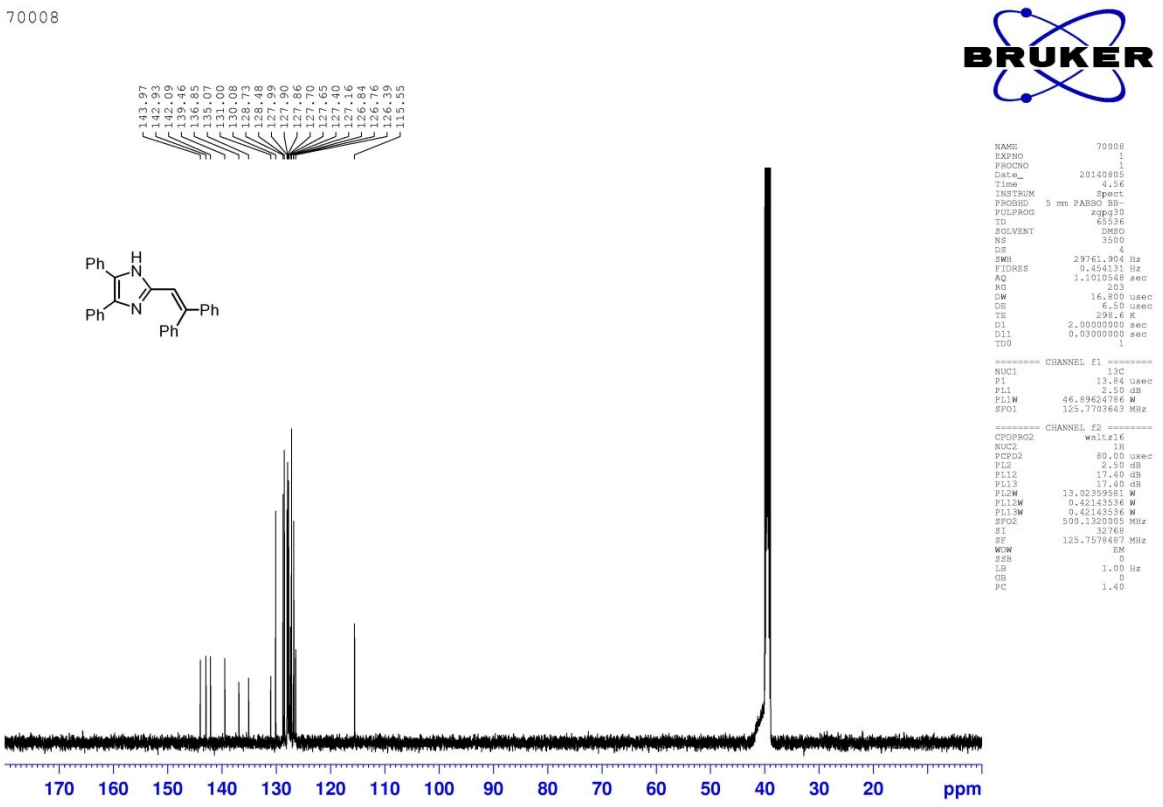
**3j**


12.596
7.555
7.536
7.501
7.484
7.458
7.440
7.406
7.318
7.300
7.282
7.236
7.218
7.201
3.869
3.711
3.354
2.500
Ph
Ph
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.87
2.04
7.07
2.02
1.07
6.04
3.00

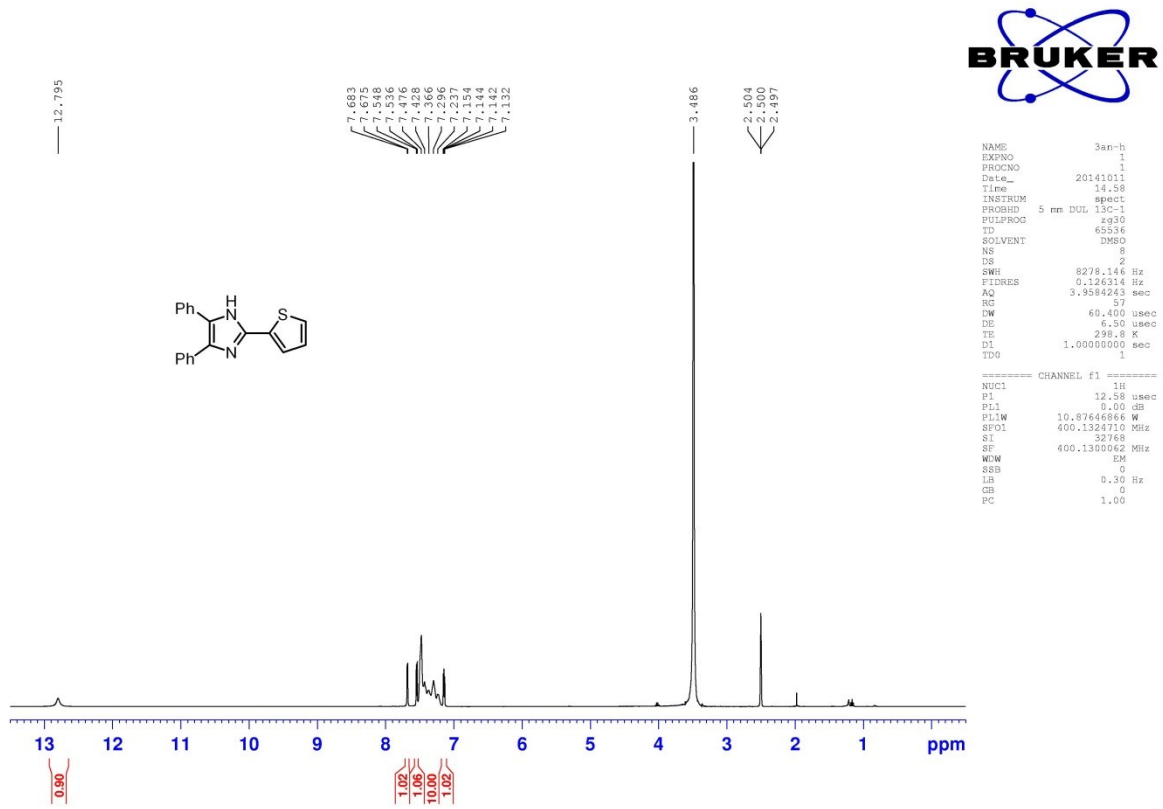

26790
153.13
145.42
137.71
136.91
135.07
131.16
128.70
128.50
128.15
128.07
127.82
127.04
126.48
125.82
102.61
60.11
56.00
40.00
39.83
39.75
39.67
39.50
39.33
39.17
39.00
Ph
Ph
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

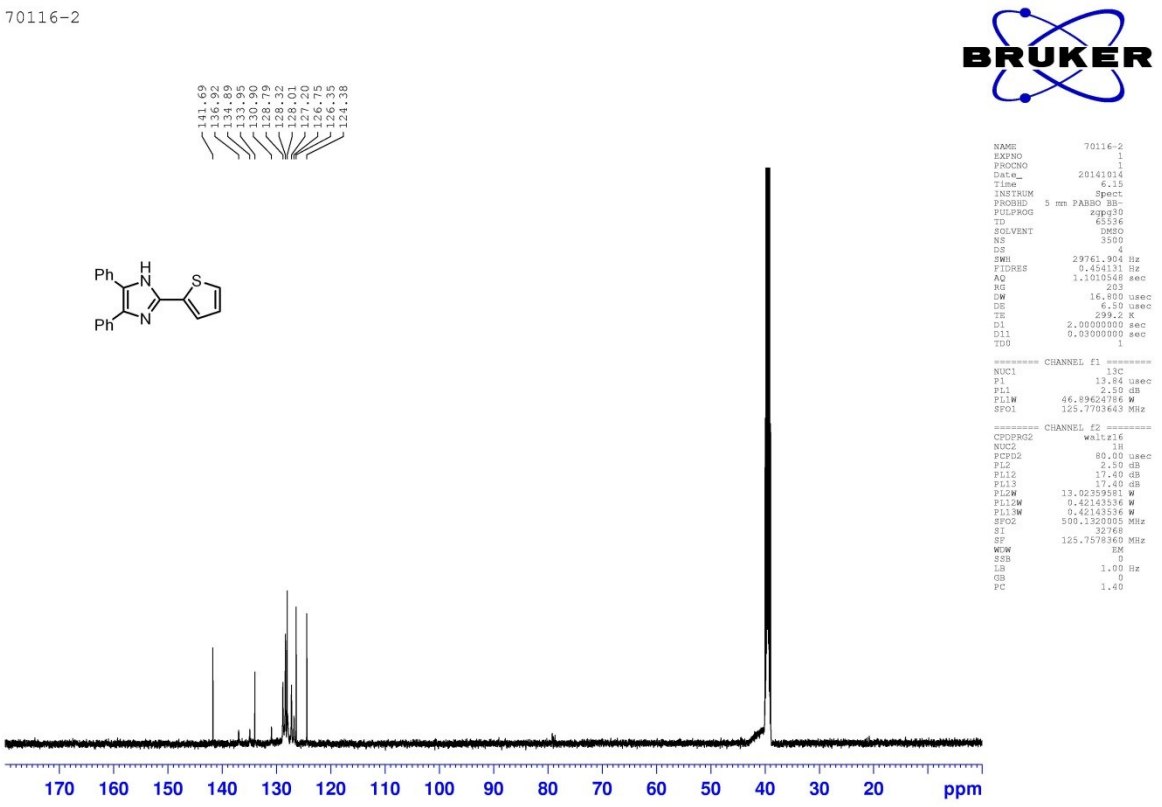
**3k**


11.810
7.443
7.427
7.408
7.387
7.367
7.330
7.305
7.283
7.208
7.191
7.172
7.155
7.138
7.120
6.900
3.368
2.500
Ph
Ph
Ph
Ph
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.94
7.08
10.00
3.05
1.02


70008
143.97
142.93
142.09
139.46
136.85
136.07
131.00
130.08
128.73
128.48
127.99
127.90
127.86
127.70
127.65
127.40
127.16
126.84
126.76
126.39
115.55
Ph
Ph
Ph
Ph
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

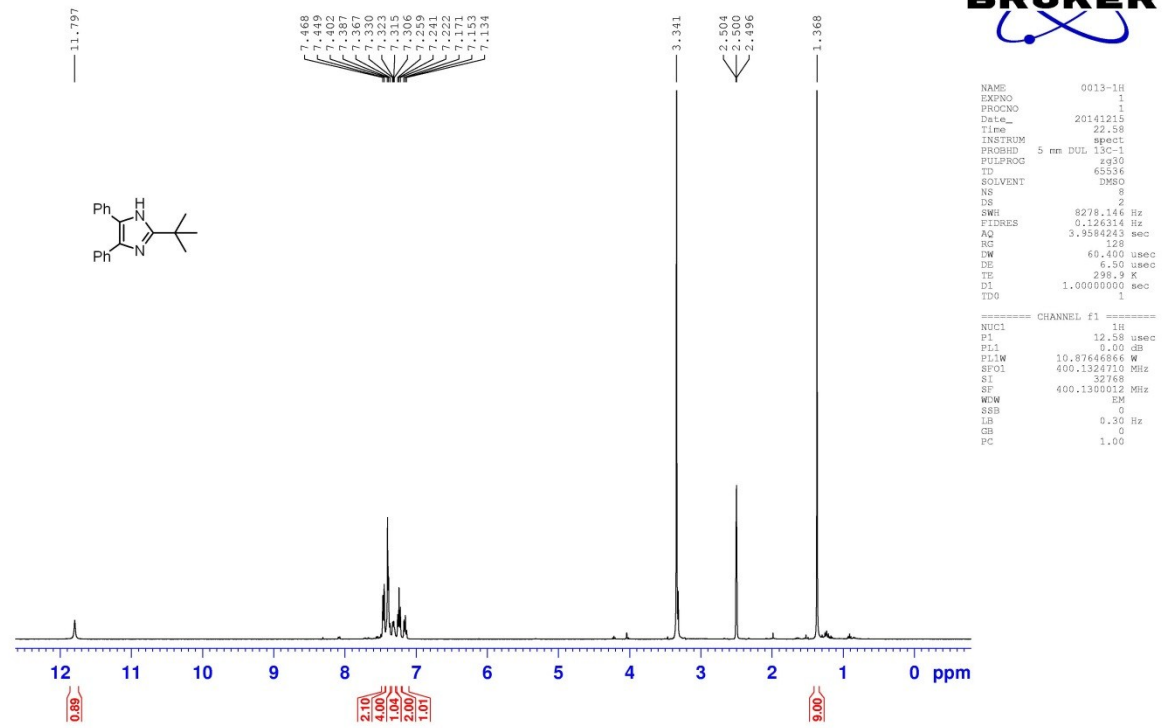
**3l**


12.795
7.683
7.675
7.548
7.536
7.476
7.428
7.366
7.296
7.237
7.154
7.144
7.142
7.132
3.486
2.504
2.500
2.497
Ph
Ph
S
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.90
1.02
1.06
10.00
1.02

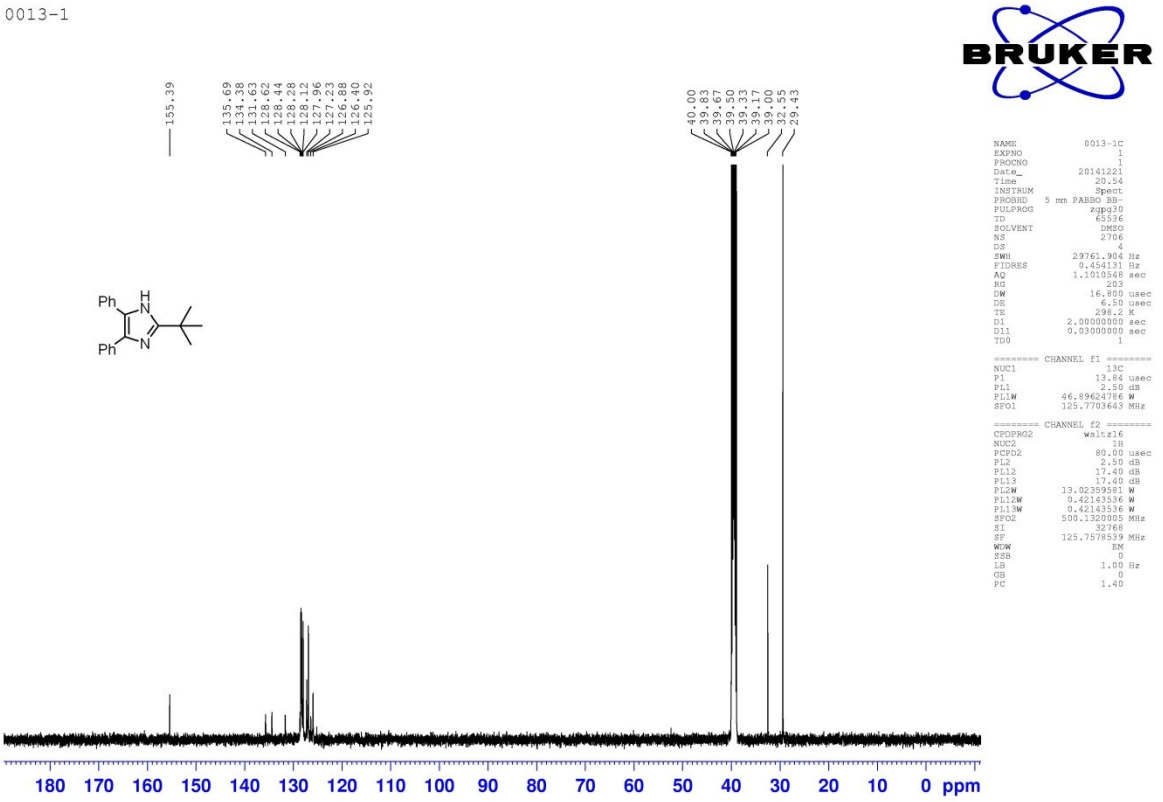



```
NAME                70116-2
EXPNO                     1
PROCNO                    1
Date_              20141014
Time                   6.15
INSTRUM                spect
PROBHD     5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                      3500
DS                         4
SWH               29761.904 Hz
FIDRES            0.454131 Hz
AQ                1.1010548 sec
RG                       203
DW                  16.800 usec
DE                   6.50 usec
TE                  299.2 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                     13.84 usec
PL1                     2.50 dB
PL1W           46.89624786 W
SFO1           125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                     1H
PCPD2                80.00 usec
PL2                     2.50 dB
PL12                   17.40 dB
PL13                   17.40 dB
PL2W           13.02359581 W
PL12W           0.42143536 W
PL13W           0.42143536 W
SFO2           500.1320005 MHz
SI                       32768
SF             125.7578360 MHz
WDW                         EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

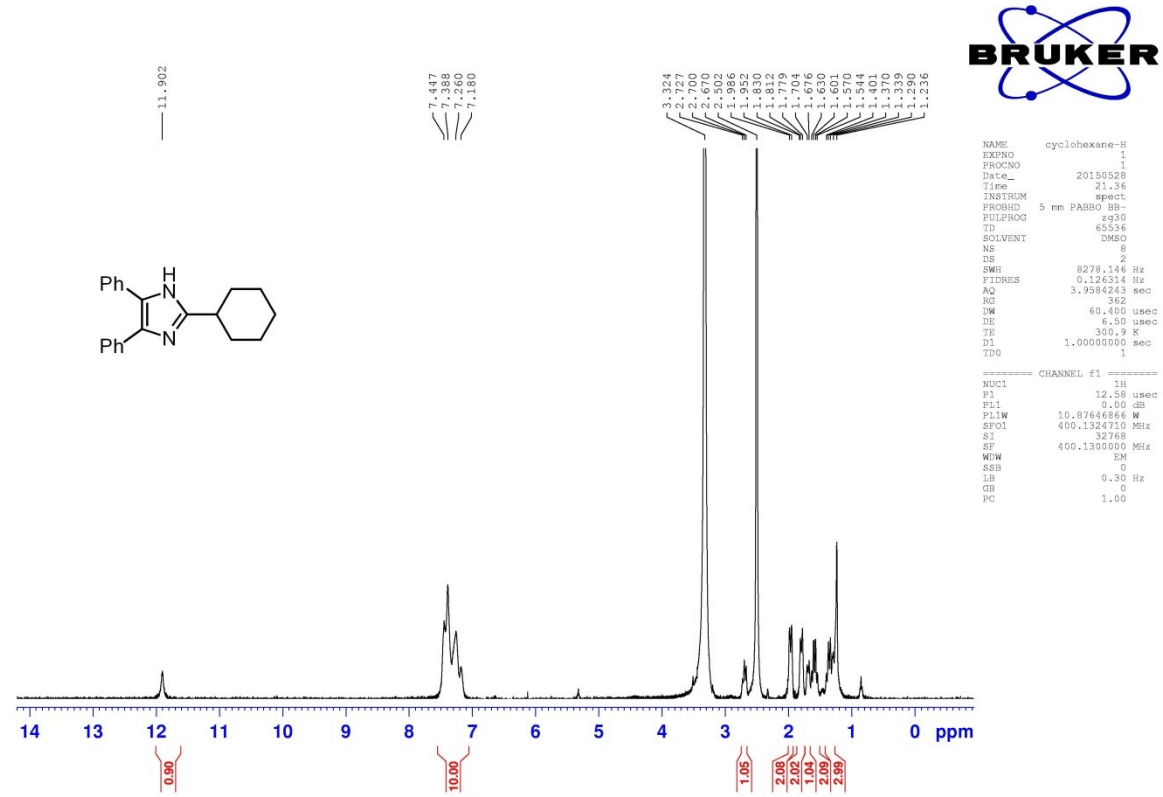
**3m**

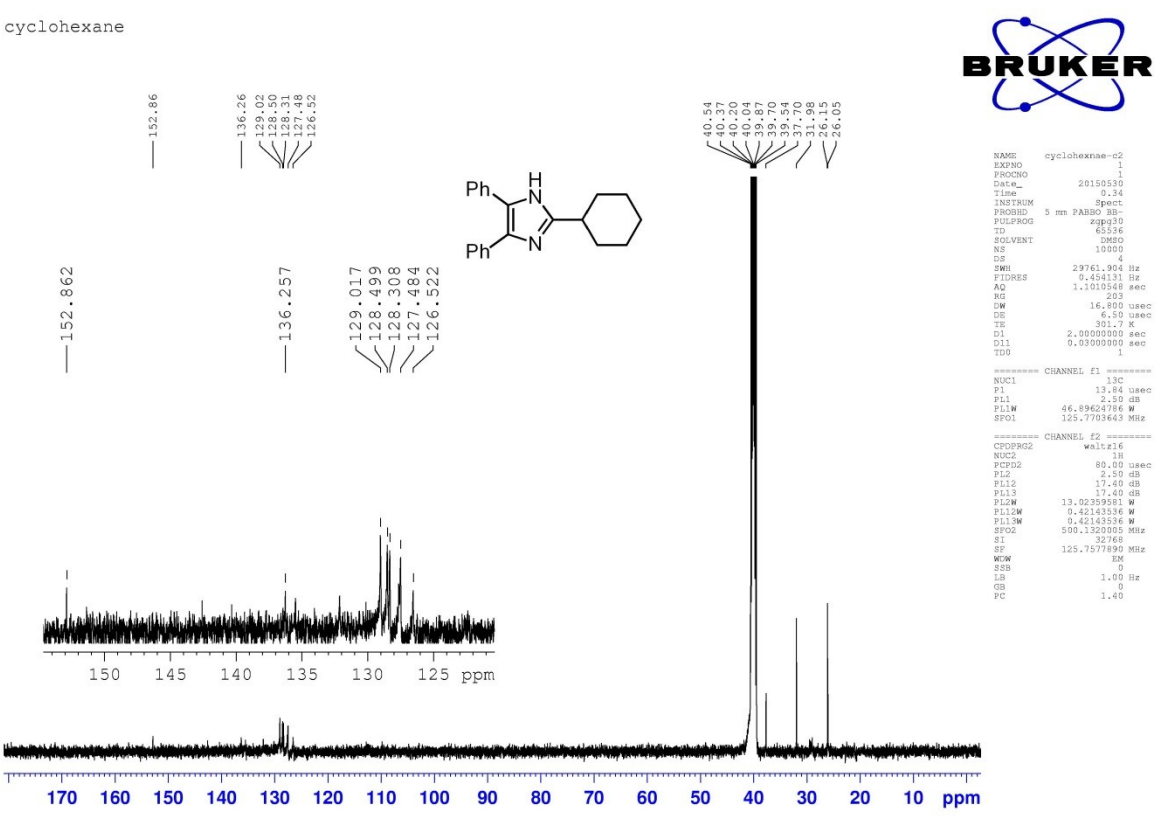



```
NAME               0013-1H
EXPNO                     1
PROCNO                    1
Date_              20141215
Time                  22.58
INSTRUM               spect
PROBHD     5 mm DUL 13C-1
PULPROG             zg30
TD                   65536
SOLVENT                DMSO
NS                         8
DS                         2
SWH                8278.146 Hz
FIDRES            0.126314 Hz
AQ                3.9584243 sec
RG                       128
DW                  60.400 usec
DE                   6.50 usec
TE                  298.9 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     1H
P1                     12.58 usec
PL1                     0.00 dB
PL1W           10.87646866 W
SFO1           400.1324710 MHz
SI                       32768
SF             400.1300012 MHz
WDW                         EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```

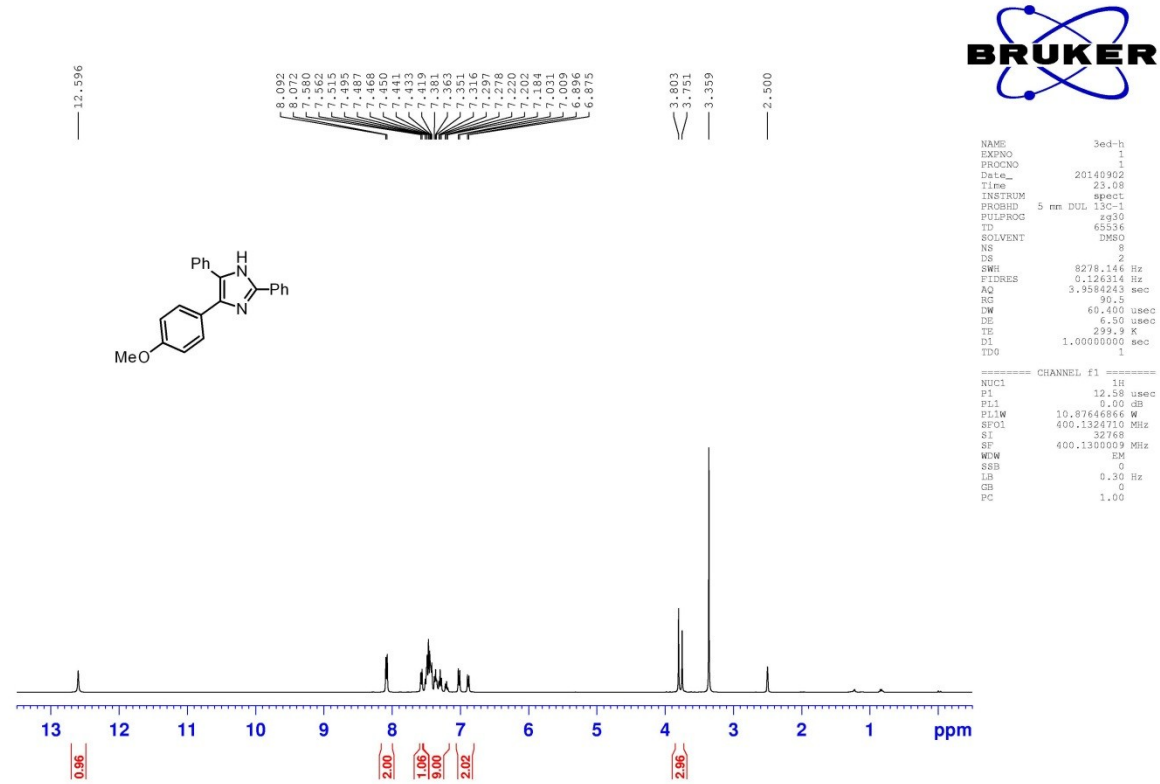

0013-1
155.39
135.69
134.38
131.63
128.62
128.24
128.18
128.12
127.96
127.23
126.88
126.40
125.92
40.00
39.83
39.67
39.50
39.33
39.17
39.00
32.55
29.43
Ph
Ph
NAME 0013-1C
EXPNO 1
PROCNO 1
Date_ 20141221
Time 20.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2706
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 13.84 usec
PL1 2.50 dB
PL1W 46.89624786 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7578539 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

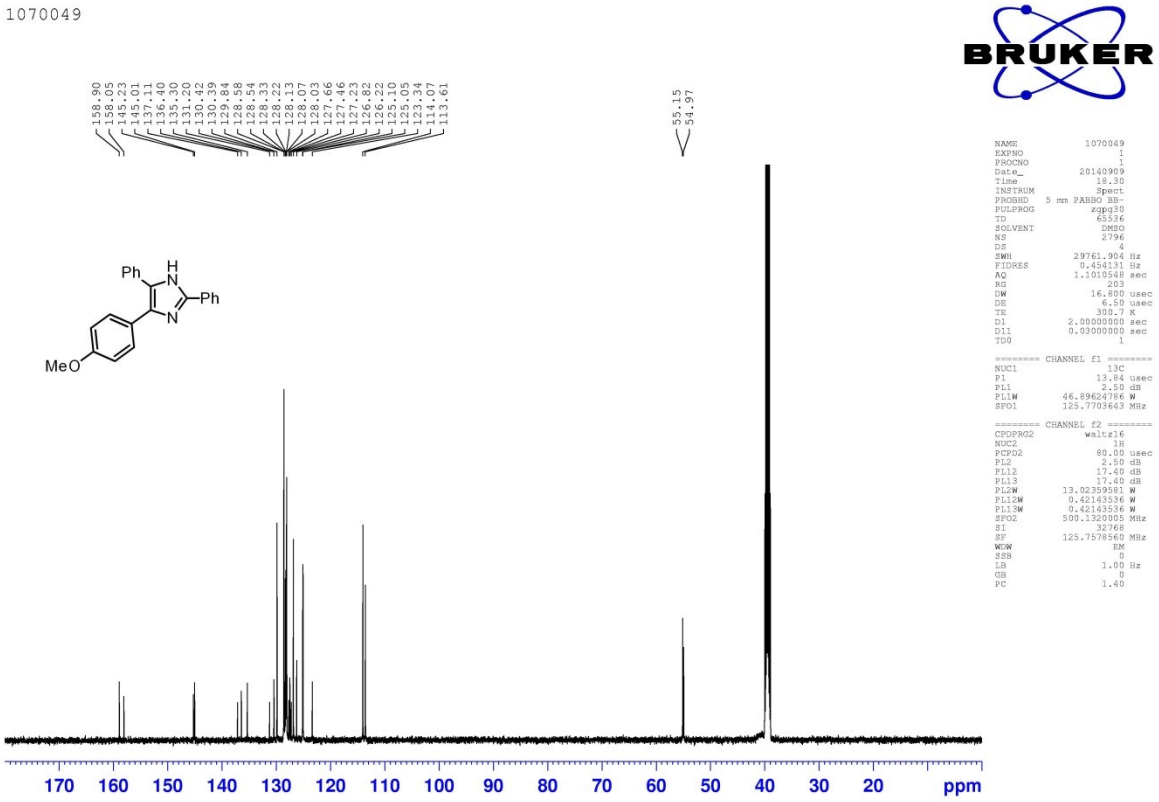
**3n**


11.902
7.447
7.388
7.260
7.180
3.324
2.727
2.700
2.670
2.502
1.986
1.952
1.830
1.812
1.779
1.704
1.676
1.630
1.601
1.570
1.544
1.401
1.370
1.339
1.290
1.236
Ph
Ph
NAME cyclohexane-H
EXPNO 1
PROCNO 1
Date_ 20150528
Time 21.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 362
DW 60.400 usec
DE 6.50 usec
TE 300.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.58 usec
PL1 0.00 dB
PL1W 10.87646866 W
SFO1 400.1326710 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.90
10.00
1.05
2.08
2.02
1.04
2.09
2.99

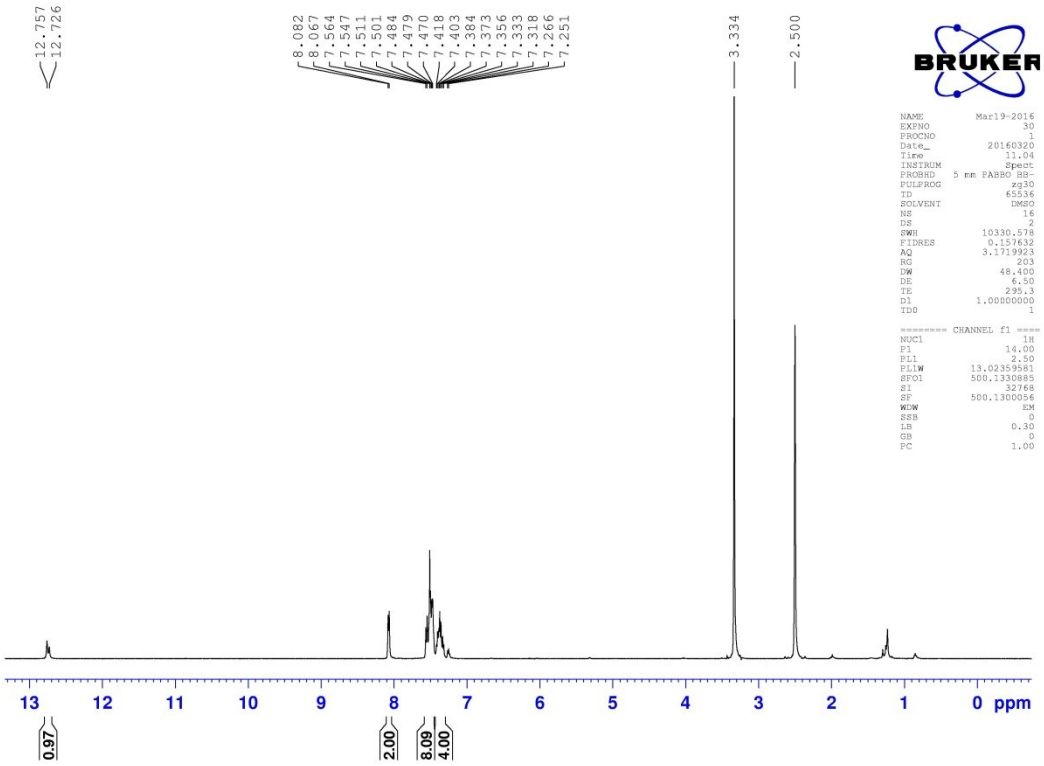

cyclohexane
152.86
136.26
129.02
128.50
128.31
127.48
126.52
40.54
40.37
40.20
40.04
39.87
39.70
39.54
37.70
31.98
26.15
26.05
Ph
Ph
152.862
136.257
129.017
128.499
128.308
127.484
126.522
150 145 140 135 130 125 ppm
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
BRUKER
NAME cyclohexnae-c2
EXPNO 1
PROCNO 1
Date_ 20150530
Time 9.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 10000
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 301.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 13.84 usec
PL1 2.50 dB
PL1W 46.89624786 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

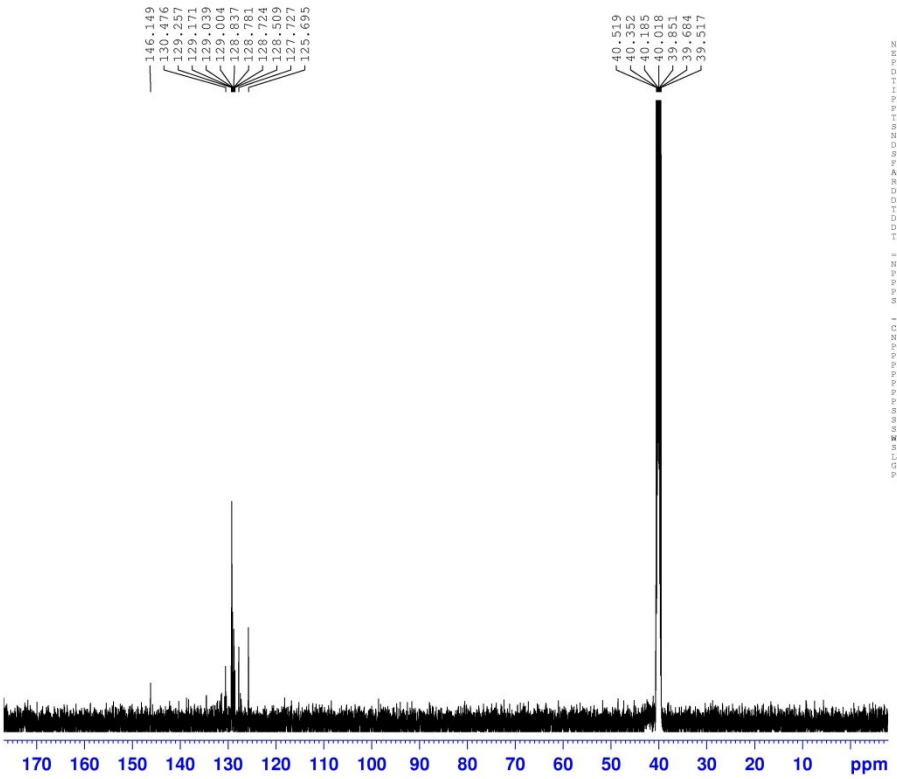
**3o**


12.596
8.092
8.072
7.580
7.562
7.515
7.495
7.487
7.468
7.450
7.441
7.433
7.419
7.381
7.363
7.351
7.316
7.297
7.278
7.220
7.202
7.184
7.031
7.009
6.896
6.875
3.803
3.751
3.359
2.500
Ph
Ph
MeO
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.96
2.00
1.06
9.00
2.02
2.96
BRUKER
NAME 3ed-h
EXPNO 1
PROCNO 1
Date_ 20140902
Time 23.08
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 90.5
DW 60.400 usec
DE 6.50 usec
TE 299.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.58 usec
PL1 0.00 dB
PL1W 10.87646866 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300009 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


1070049
158.90
158.05
145.23
145.01
137.11
136.40
135.30
131.20
130.42
130.39
129.84
128.58
128.34
128.33
128.22
128.13
128.07
128.03
127.66
127.46
127.23
126.82
126.22
125.10
123.95
123.34
114.07
113.61
55.15
54.97
Ph
H
N
Ph
N
MeO
NAME 1070049
EXPNO 1
PROCNO 1
Date_ 20140909
Time 18.30
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2796
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 300.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 13.84 usec
PL1 2.50 dB
PL1W 46.89624786 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7578560 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

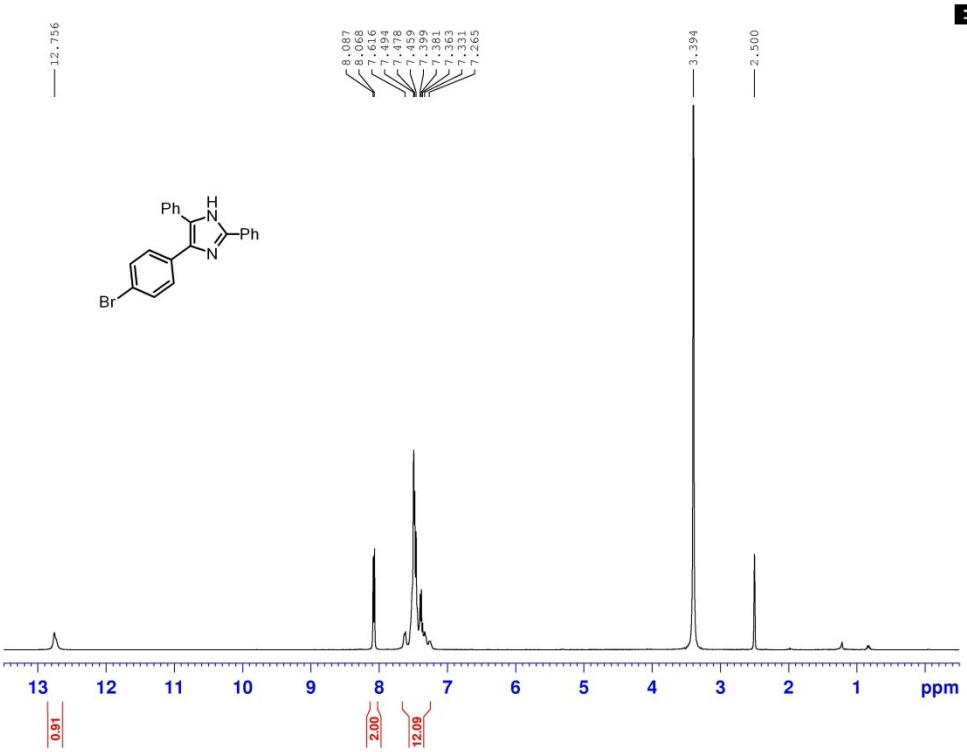
3p


12.757
12.726
8.082
8.067
7.564
7.547
7.511
7.501
7.484
7.479
7.470
7.418
7.403
7.384
7.373
7.356
7.333
7.318
7.266
7.251
3.334
2.500
NAME Mar19-2016
EXPNO 30
PROCNO 1
Date_ 20160320
Time 11.04
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578
FIDRES 0.157632
AQ 3.1719923
RG 203
DW 48.400
DE 6.50
TE 295.3
D1 1.00000000
TD0 1
======== CHANNEL f1 ====
NUC1 1H
P1 14.00
PL1 2.50
PL1W 13.02359581
SFO1 500.1330885
SI 32768
SF 500.1300056
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00
13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.97
2.00
8.09
4.00

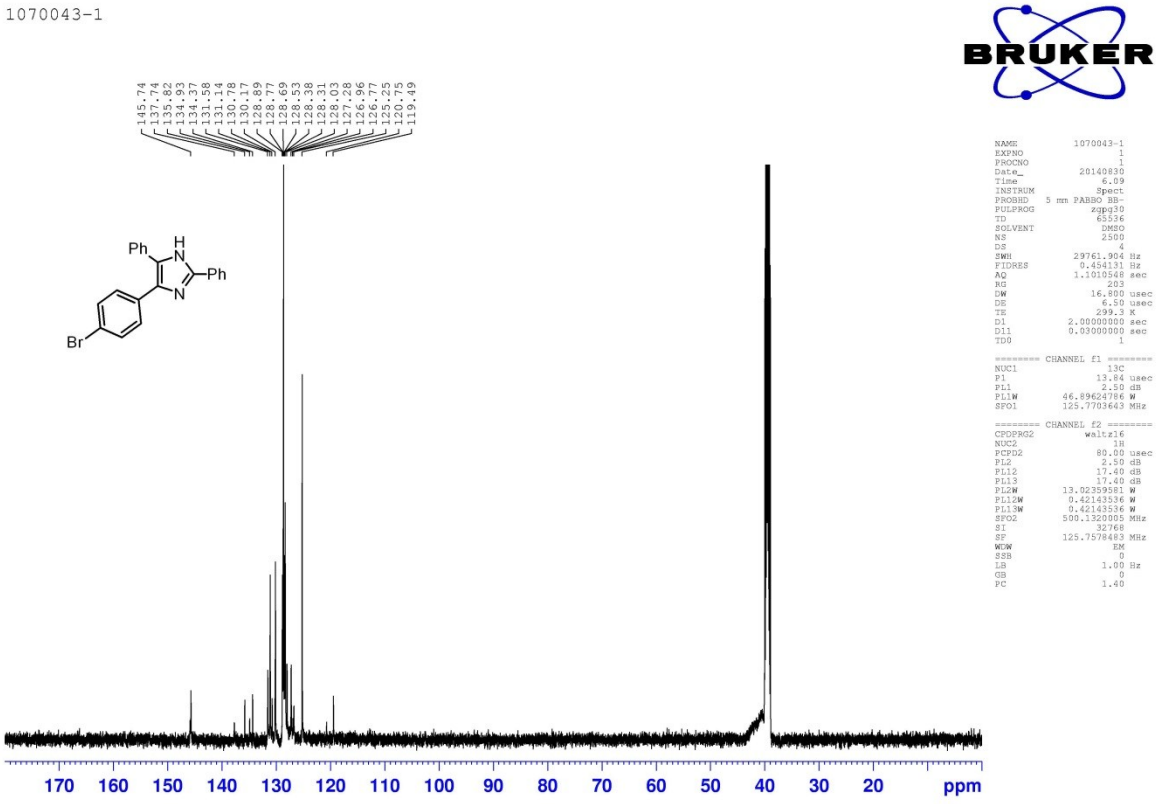



```
NAME            Mar19-2016
EXPNO                   31
PROCNO                   1
Date_             20160320
Time                 11.59
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                  65536
SOLVENT              DMSO
NS                    1024
DS                       4
SWH              29761.904 Hz
FIDRES           0.454131 Hz
AQ               1.1010548 sec
RG                     203
DW                  16.800 usec
DE                   6.50 usec
TE                  297.6 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                   13.84 usec
PL1                   2.50 dB
PL1W          46.89624786 W
SFO1          125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                   2.50 dB
PL12                 17.40 dB
PL13                 17.40 dB
PL2W          13.02359581 W
PL12W          0.42143536 W
PL13W          0.42143536 W
SFO2          500.1320005 MHz
SI                   32768
SF            125.7577890 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

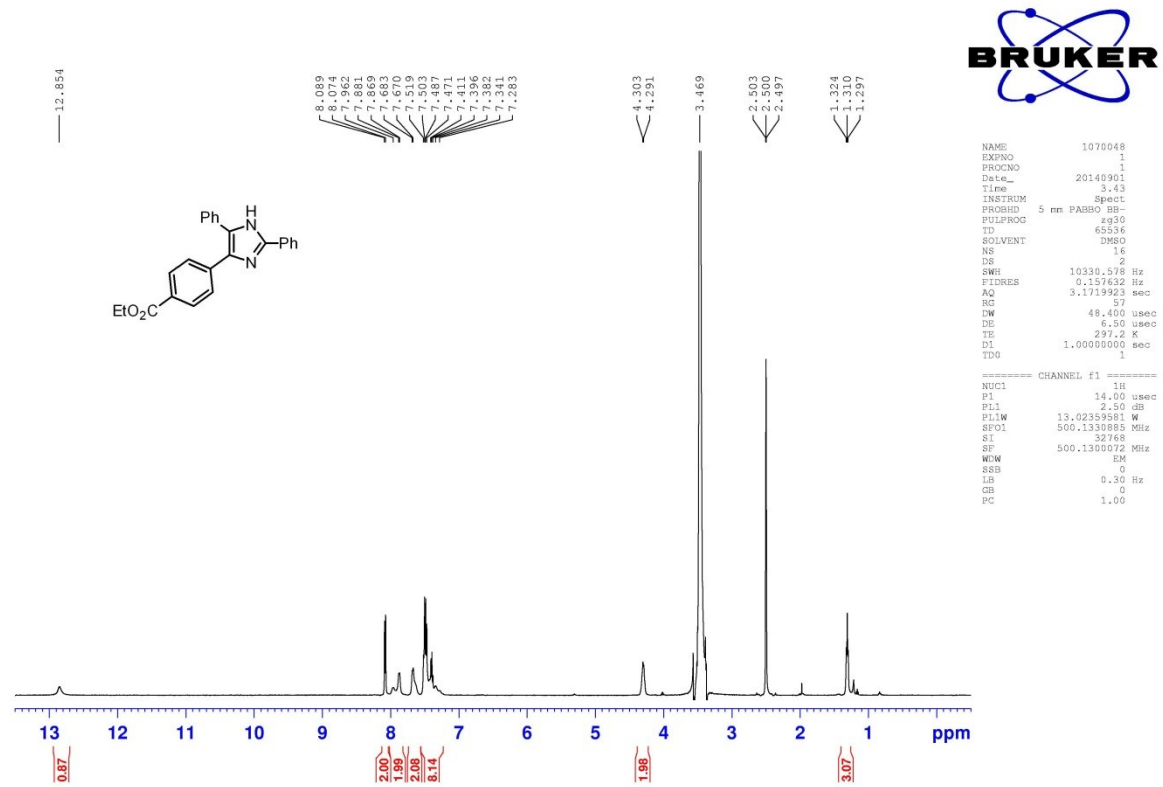
**3q**

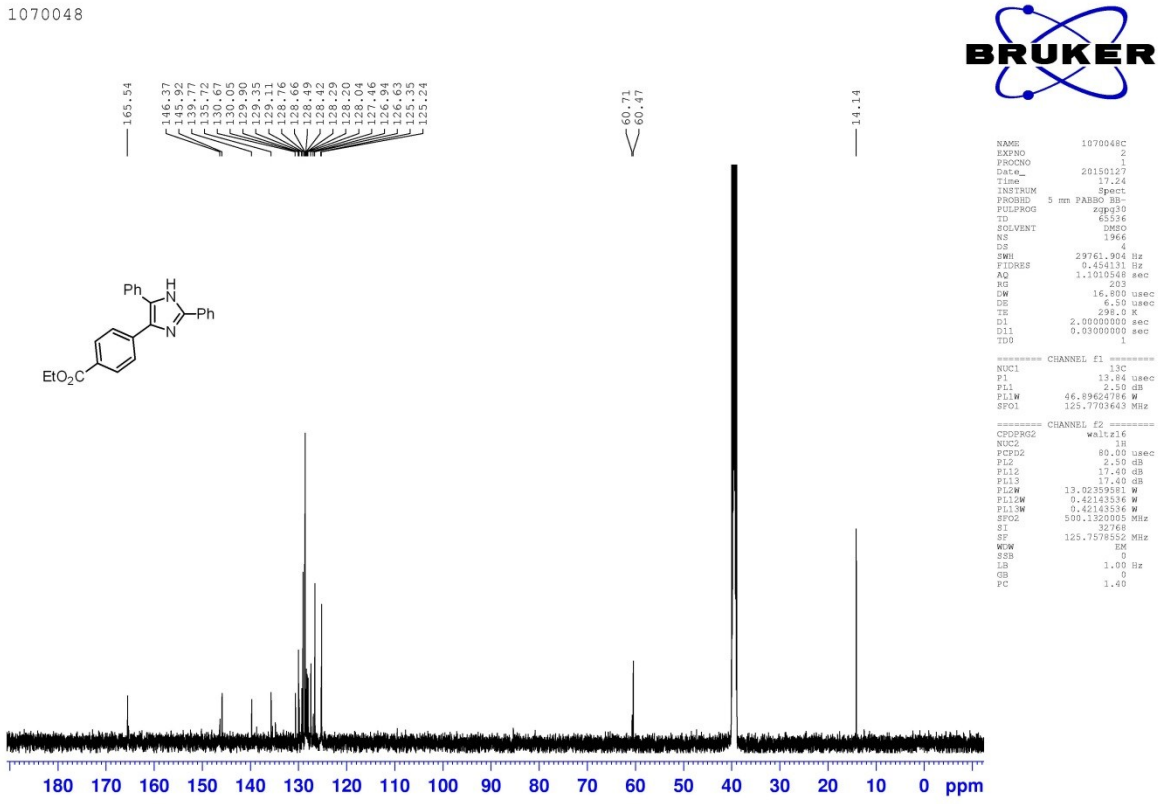



```
NAME                 3fd-h
EXPNO                    1
PROCNO                   1
Date_             20140829
Time                 21.49
INSTRUM              spect
PROBHD   5 mm DUL 13C-1
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                       8
DS                       2
SWH               8278.146 Hz
FIDRES           0.126314 Hz
AQ               3.9584243 sec
RG                    71.8
DW                  60.400 usec
DE                   6.50 usec
TE                  300.0 K
D1               1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   1H
P1                   12.58 usec
PL1                   0.00 dB
PL1W          10.87646866 W
SFO1          400.1324710 MHz
SI                   32768
SF            400.1300008 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

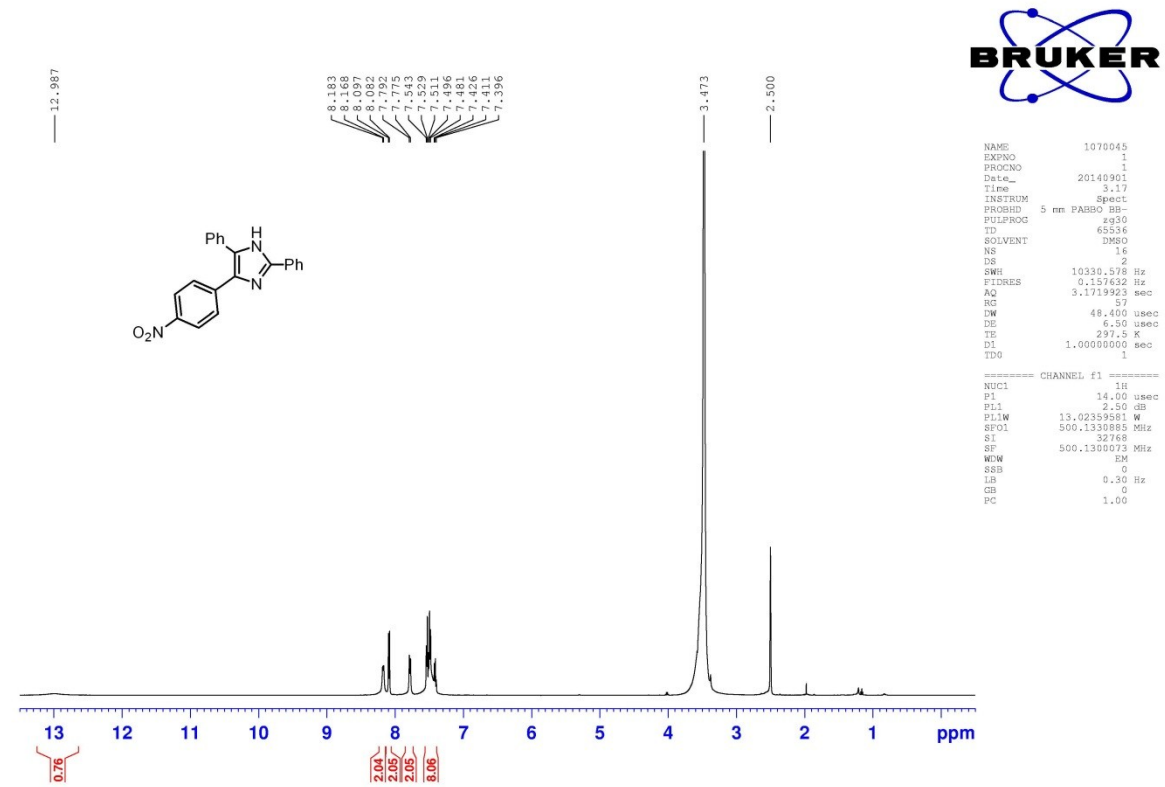

1070043-1
145.74
137.74
135.82
134.43
134.37
131.58
131.14
130.78
130.17
128.89
128.77
128.69
128.53
128.38
128.31
128.03
127.28
126.96
126.77
125.25
120.75
119.49
Ph
H
N
Ph
N
Br
NAME 1070043-1
EXPNO 1
PROCNO 1
Date_ 20140830
Time 6.09
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2500
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 299.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 13.84 usec
PL1 2.50 dB
PL1W 46.89624786 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7578483 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

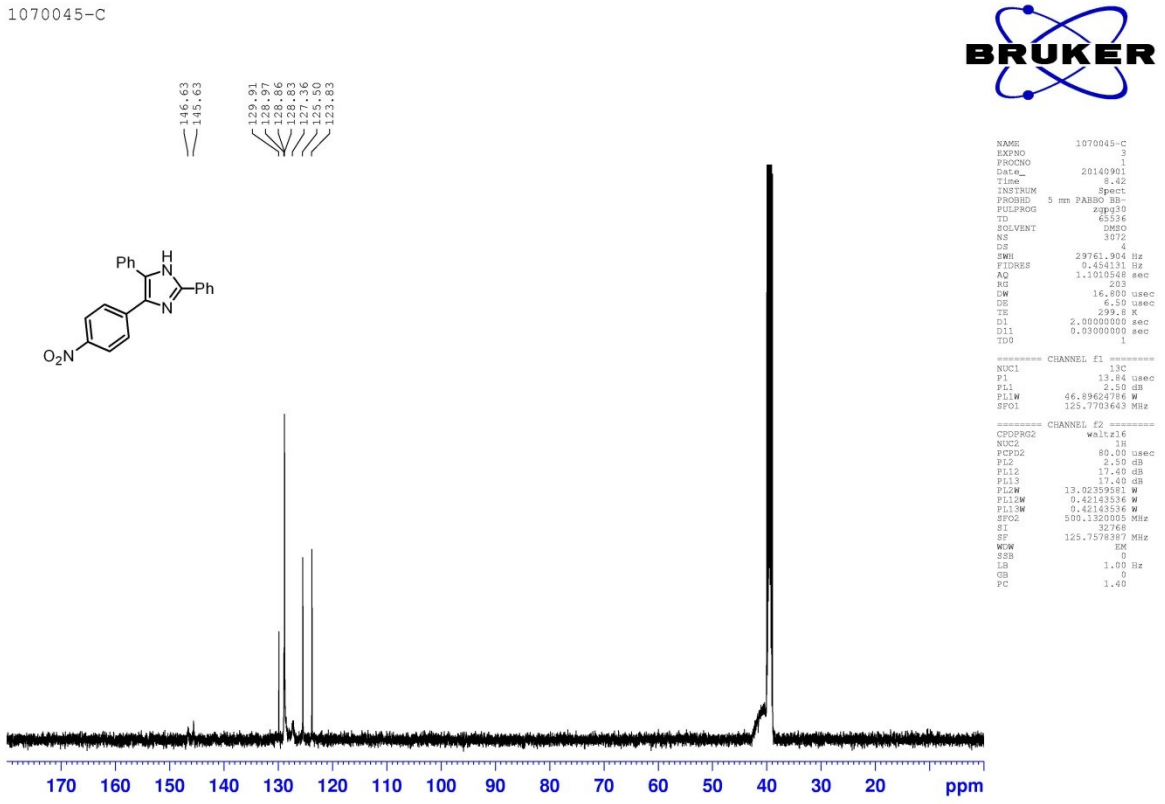
**3r**


12.854
8.089
8.074
7.962
7.881
7.869
7.683
7.670
7.519
7.503
7.487
7.471
7.411
7.396
7.382
7.341
7.283
4.303
4.291
3.469
2.503
2.500
2.497
1.324
1.310
1.297
Ph
H
N
Ph
N
EtO2C
NAME 1070048
EXPNO 1
PROCNO 1
Date_ 20140901
Time 3.43
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 57
DW 48.400 usec
DE 6.50 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 2.50 dB
PL1W 13.02359581 W
SFO1 500.1330885 MHz
SI 32768
SF 500.1300072 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.87
2.00
1.99
2.08
8.14
1.98
3.07

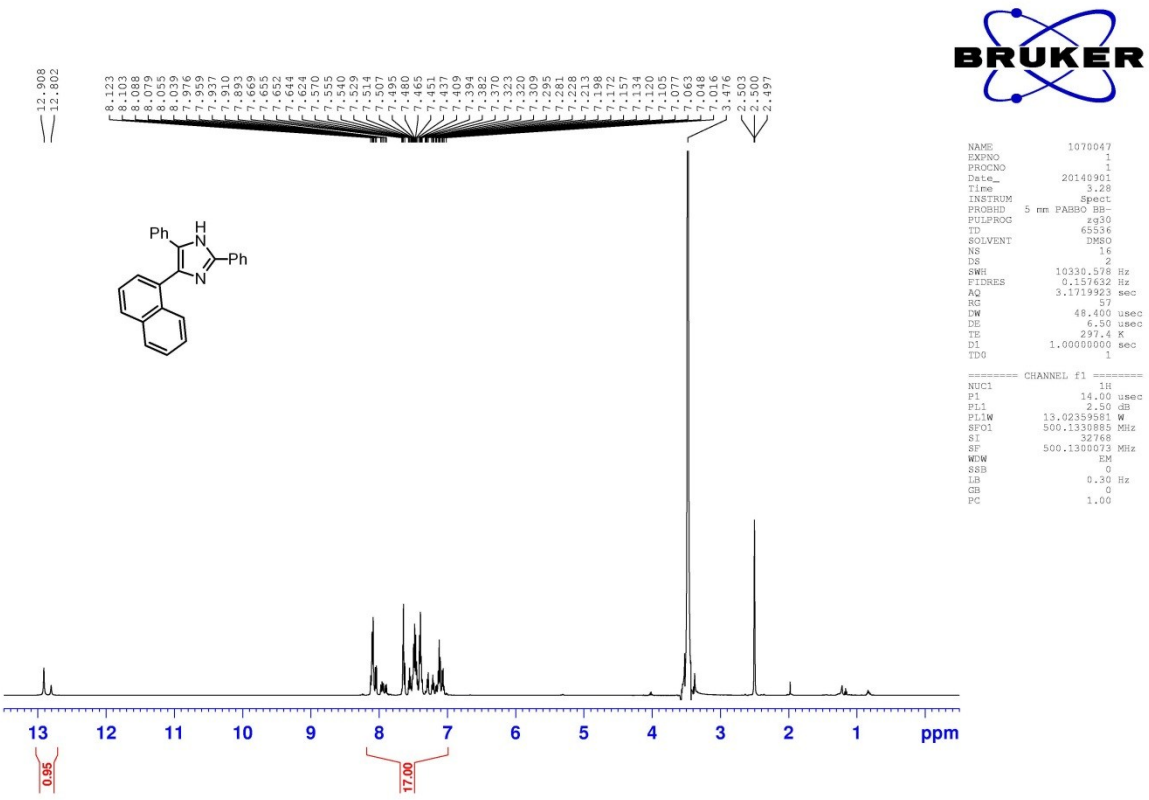

1070048
BRUKER
165.54
146.37
145.92
139.77
135.72
130.67
130.05
129.90
129.35
129.11
128.76
128.66
128.49
128.42
128.29
128.20
128.04
127.46
126.94
126.63
125.35
125.24
60.71
60.47
14.14
Ph
N
H
N
Ph
EtO2C
NAME 1070048c
EXPNO 2
PROCNO 1
Date_ 20150127
Time 17.24
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1966
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 13.84 usec
PL1 2.50 dB
PL1W 46.89624786 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7578552 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

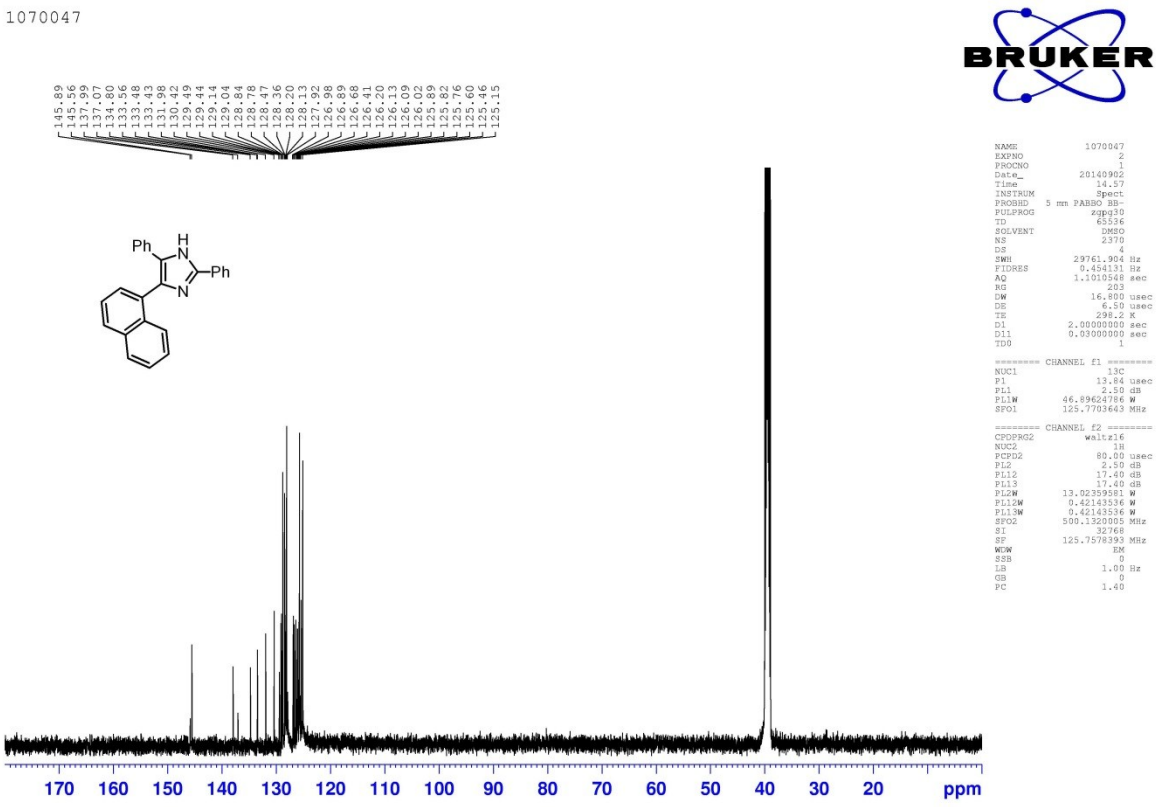
**3s**


BRUKER
12.987
8.183
8.168
8.097
8.082
7.792
7.775
7.543
7.529
7.511
7.496
7.481
7.426
7.411
7.396
3.473
2.500
Ph
N
H
N
Ph
O2N
NAME 1070045
EXPNO 1
PROCNO 1
Date_ 20140901
Time 3.17
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 57
DW 48.400 usec
DE 6.50 usec
TE 297.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 2.50 dB
PL1W 13.02359581 W
SFO1 500.1330885 MHz
SI 32768
SF 500.1300073 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.76
2.04
2.05
2.05
8.06

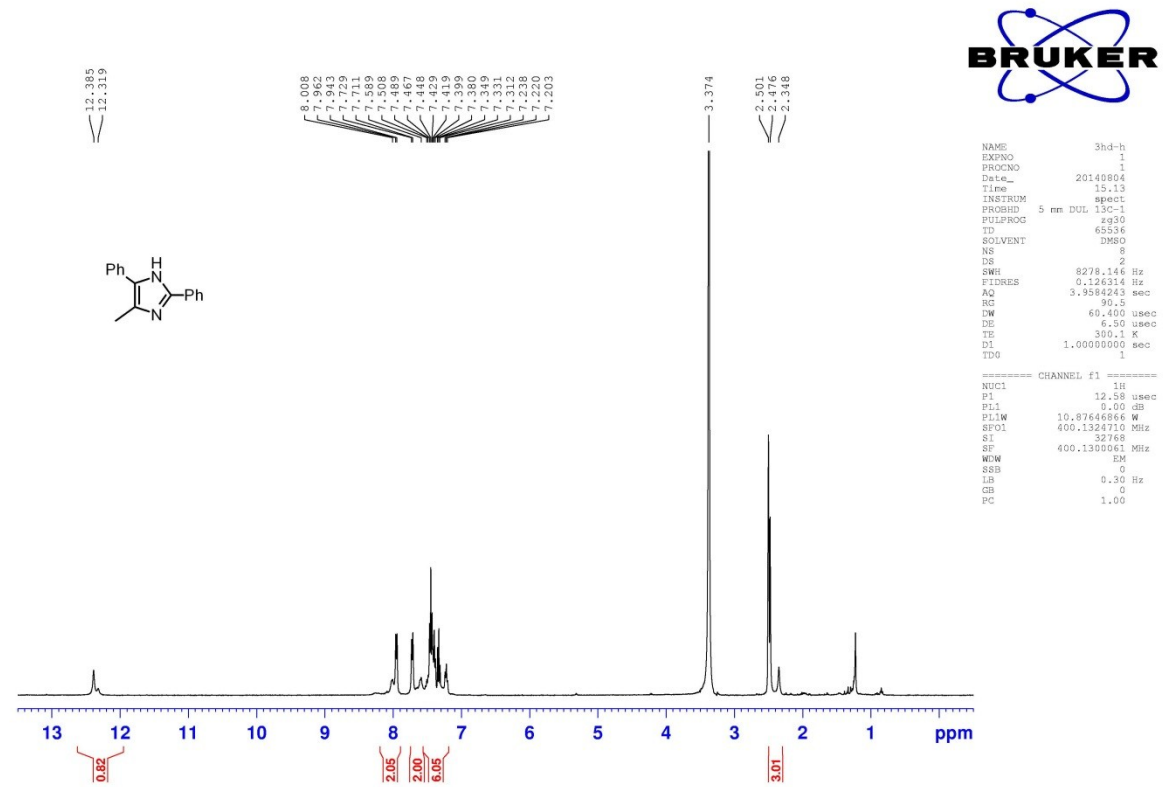

1070045-C
146.63
145.63
129.91
128.97
128.86
128.83
127.36
125.50
123.83
Ph
H
N
Ph
N
$O_2N$
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm
NAME 1070045-C
EXPNO 3
PROCNO 1
Date_ 20140901
Time 8.42
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 3072
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 13.84 usec
PL1 2.50 dB
PL1W 46.89624786 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7578387 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

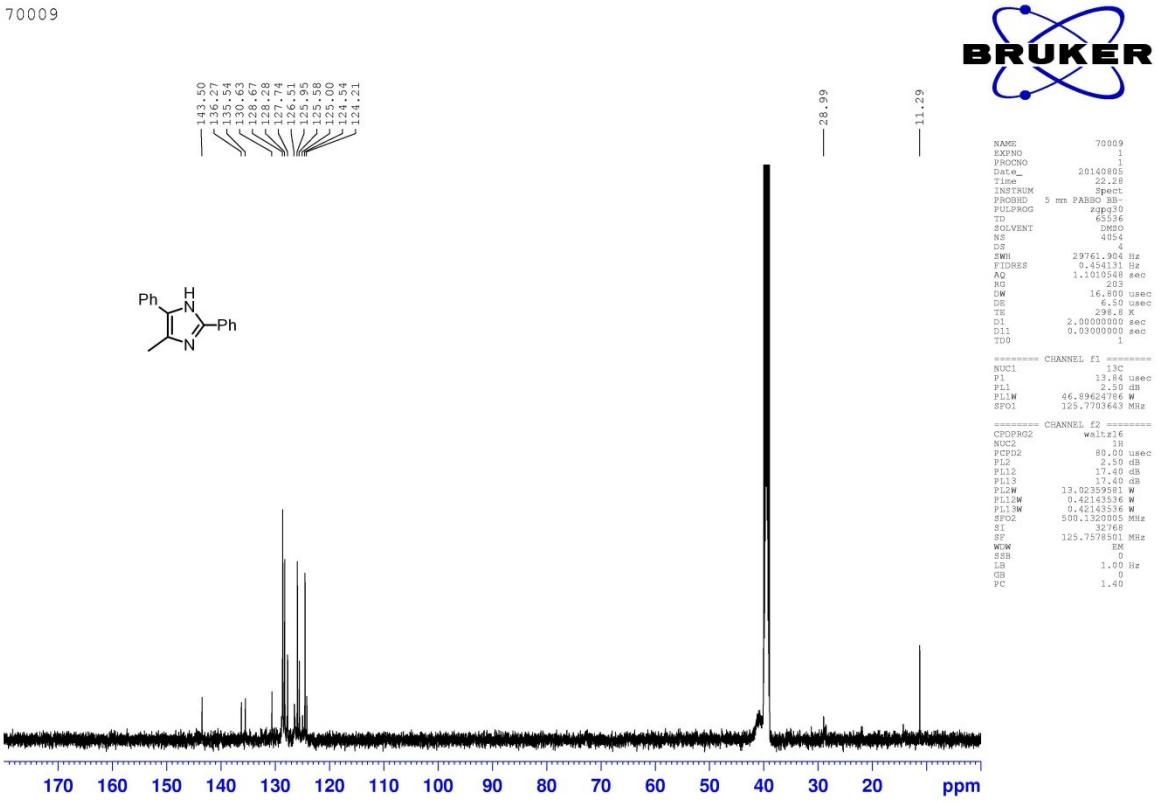
**3t**


12.908
12.802
8.123
8.103
8.088
8.079
8.055
8.039
7.976
7.959
7.937
7.910
7.893
7.669
7.655
7.652
7.644
7.624
7.570
7.555
7.540
7.529
7.514
7.507
7.495
7.480
7.465
7.451
7.437
7.409
7.394
7.382
7.370
7.323
7.320
7.309
7.295
7.281
7.228
7.213
7.198
7.172
7.157
7.134
7.120
7.105
7.077
7.063
7.048
7.016
3.476
2.503
2.500
2.497
Ph
H
N
Ph
N
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.95
17.00
NAME 1070047
EXPNO 1
PROCNO 1
Date_ 20140901
Time 3.28
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 57
DW 48.400 usec
DE 6.50 usec
TE 297.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 2.50 dB
PL1W 13.02359581 W
SFO1 500.1330885 MHz
SI 32768
SF 500.1300073 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


1070047
BRUKER
145.89
145.56
137.99
137.07
134.80
133.56
133.48
133.43
131.98
130.42
129.49
129.44
129.14
129.04
128.84
128.78
128.37
128.36
128.20
128.13
127.92
126.98
126.89
126.68
126.41
126.20
126.13
126.09
126.02
125.89
125.82
125.76
125.60
125.46
125.15
Ph
H
N
Ph
N
NAME 1070047
EXPNO 2
PROCNO 1
Date_ 20140902
Time 14.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2370
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 13.84 usec
PL1 2.50 dB
PL1W 46.89624786 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7578393 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

**3u**


12.385
12.319
8.008
7.962
7.943
7.729
7.711
7.589
7.508
7.489
7.467
7.448
7.429
7.419
7.399
7.380
7.349
7.331
7.312
7.238
7.220
7.203
3.374
2.501
2.476
2.348
BRUKER
Ph
H
N
Ph
N
NAME 3hd-h
EXPNO 1
PROCNO 1
Date_ 20140804
Time 15.13
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 90.5
DW 60.400 usec
DE 6.50 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.58 usec
PL1 0.00 dB
PL1W 10.87646866 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300061 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.82
2.05
2.00
6.05
3.01


70009
143.50
136.27
135.54
130.63
128.67
128.28
127.74
126.51
125.95
125.58
125.00
124.54
124.21
28.99
11.29
Ph
H
N
N
Ph
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm
NAME 70009
EXPNO 1
PROCNO 1
Date_ 20140805
Time 22.28
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4054
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 298.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 13.84 usec
PL1 2.50 dB
PL1W 46.89624786 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7578501 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40