Au-Catalyzed Skeletal Rearrangement of *O*-Propargylic Oximes via N-O Bond Cleavage with the Aid of a Brønsted Base Cocatalyst

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Supporting Information

Contents

1. General information

^{1}H and ^{13}C NMR spectra were recorded on JEOL JNM-ECS400 (400 MHz for ^{1}H and 100 MHz for ^{13}C) spectrometer. Chemical shifts are reported in ppm relative to $CHCl_3$ (for ^{1}H, δ 7.26), and $CDCl_3$ (for ^{13}C, δ 77.00). ^{1}H NMR data are reported as follows: chemical shift, integration, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, sext = sextet, sep = septet, br = broad, m = multiplet) and coupling constants (Hz). Infrared (IR) spectra were recorded on a JASCO FT/IR- 4100 spectrometer. High-resolution mass spectra analysis was performed on a Bruker Daltonics APEX III FT-ICR-MS spectrometer and Bruker Daltonics solariX FT-ICR-MS spectrometer at Research and Analytical Center for Giant Molecules, Graduate School of Science, Tohoku University. Melting points (Mp) were measured by METTLER TOLEDO MP70. Flash column chromatography was performed on silica gel 60N (Merck 40-63 μm or Kanto 40-50 μm). Analytical thin layer chromatography (TLC) was performed on Merck pre-coated TLC plates (silica gel 60 F254).

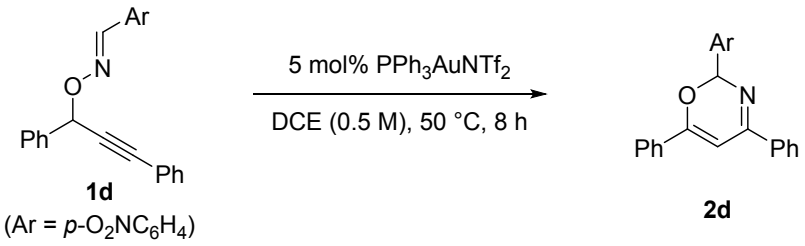
Materials

Anhydrous dichloromethane was purchased form KANTO Chemical Co., Inc., anhydrous 1,2-dichloroethane (DCE) was purchased from Sigma-Aldrich, and anhydrous pyridine was purchased from WAKO. These reagents were used as received. Substrates **1** were synthesized in accordance with the literature method.[1] PPh_3AuNTf_2 was prepared from PPh_3AuCl and $AgNTf_2$ in accordance with the literature method reported by Gagosz *et al*.[2] PPh_3AuCl and $AgNTf_2$ were purchased from WAKO and from KANTO Chemical Co., Inc., respectively. $CDCl_3$ was purchased from KANTO Chemical Co., Inc.. All air- and moisture-sensitive manipulations were performed under argon atmosphere using oven-dried glassware, including standard Schlenk and glovebox techniques. All reactions were carried out under argon atmosphere.

[1] Nakamura, I.; Kudo, Y.; Araki, T.; Zhang, D.; Kwon, E.; Terada, M. Synthesis., 2012, **44**, 1542 Supporting Information:
www.thieme-connect.com/media/synthesis/201210/supmat/sup_ss-2012-c0227-st_10-1055_s-0031-1290819.pdf

[2] Mézailles, N.; Ricard, L.; Gagosz, F. *Org. Lett.*, 2005, **7**, 4133

2. General procedure for the Au-catalyzed reaction of 1



1d
(Ar = *p*-$O_2NC_6H_4$)

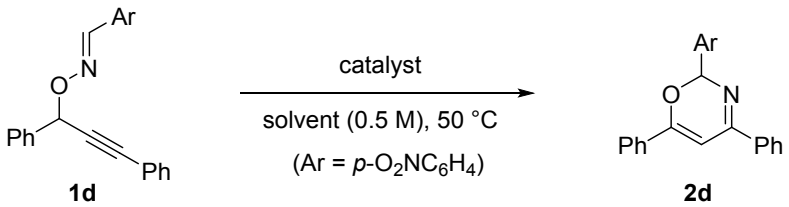
2d

To a solution of **1d** (71.3 mg, 0.2 mmol) in DCE (0.4 mL) in a V-vial under argon atmosphere was added PPh_3AuNTf_2 (7.4 mg, 0.01 mmol). The resulting mixture was stirred at 50 °C for 8 h, then passed through a short pad of silica gel with CH_2Cl_2 (50 mL). After removing the solvents *in vacuo*, the crude product was purified using flash silica-gel column chromatography with hexane/EtOAc [5/1 (v/v)] as eluent to afford product **2d** (0.19 mmol 66.3 mg, 93%) in an analytically pure form.

It should be noted that hexane/EtOAc [5/1 (v/v)] was used as eluent for silica gel column chromatography for purification of all products **2**. Reaction time and R_f value are reported in Section 11.

3. Optimization of reaction conditions

Table S1. Screening of Catalyst and Solvent.

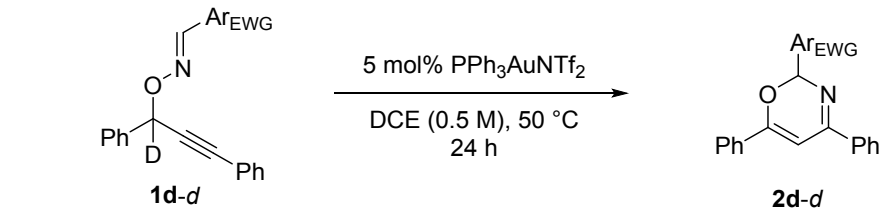


1d **2d**

	catalyst (mol%)	solvent	time (h)	**2d** (%)[a]
1	AuCl (10)	DCE	8	80
2	AuCl (5), $AgNTf_2$ (5)	DCE	8	52
3	$AuCl_3$ (5)	DCE	50	<1
4	$AgNTf_2$ (5)	DCE	24	<1
5	$PtCl_2$ (10)	DCE	24	<1
6	CuCl (10)	DCE	48	<1
7	PPh_3AuNTf_2 (5)	DCE	8	(93)
8	[P(*p*-$F_3CC_6H_4)_3$]$AuNTf_2$ (5)	DCE	8	88
9	[P(*p*-$FC_6H_4)_3$]$AuNTf_2$ (5)	DCE	8	89
10	[P(*p*-$MeOC_6H_4)_3$]$AuNTf_2$ (5)	DCE	8	91
11	PCy_3AuNTf_2 (5)	DCE	8	87
12	$IPrAuNTf_2$ (5)	DCE	8	54
13	$SPhosAuNTf_2$ (5)	DCE	8	62
14	PPh_3AuCl (5), AgOAc (5)	DCE	24	18
15	PPh_3AuCl (5), AgOTf (5)	DCE	8	56
16	PPh_3AuCl (5), AgOTs (5)	DCE	8	85
17	PPh_3AuNTf_2 (5)	CH_3CN	8	84
18	PPh_3AuNTf_2 (5)	DMF	8	87
19	PPh_3AuNTf_2 (5)	THF	12	83
20	PPh_3AuNTf_2 (5)	toluene	12	83
21	PPh_3AuNTf_2 (5)	DMSO	24	92
19	PPh_3AuNTf_2 (5)	CH_3OH	8	<1

[a] The yields were determined by ^1H NMR using dibromomethane as an internal standard. Isolated yields in the parentheses.

4. Labeling experiments



1d-*d*
(Ar$_{EWG}$ = *p*-O$_2$NC$_6$H$_4$, >99% D)

2d-*d*
60% (85% D)

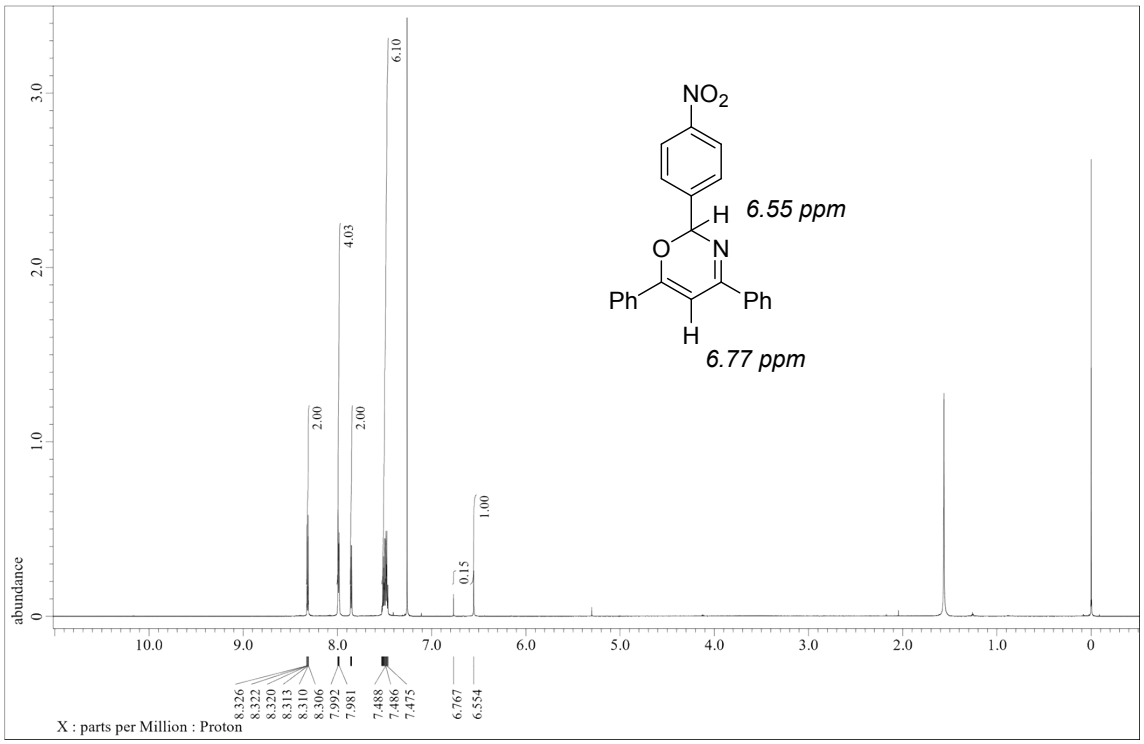
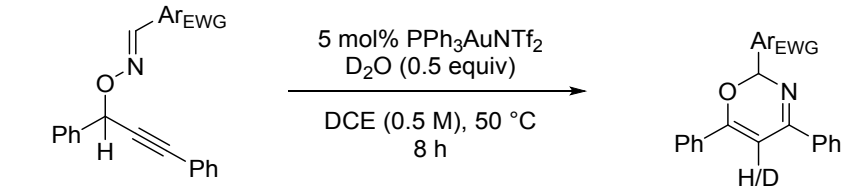


Figure S1. ^{1}H NMR chart of 2d-*d*.



1d
(Ar$_{EWG}$ = *p*-O$_2$NC$_6$H$_4$)

2d
86% (24% D)

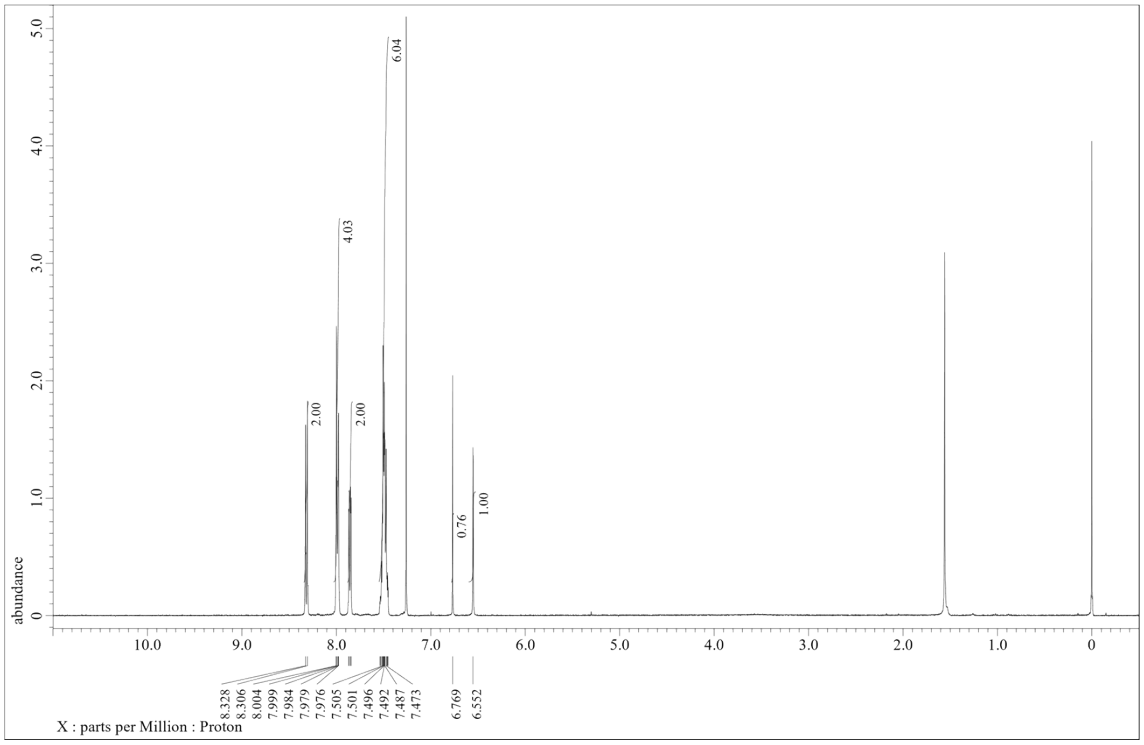
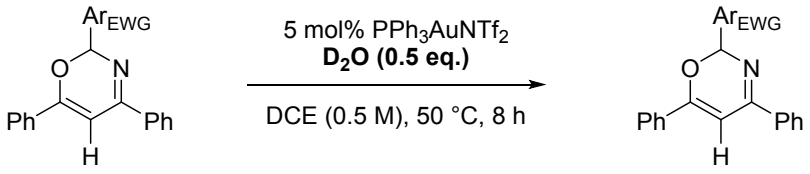


Figure S2. ^{1}H NMR chart of 2d.

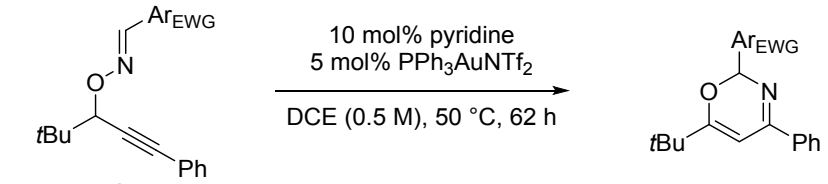


2d
(Ar$_{EWG}$ = *p*-O$_2$NC$_6$H$_4$)

2d
81% (<1% D)

Incorporation of deuterium was not observed.

5. General procedure for the Au/pyridine-cocatalyzed reaction of 1



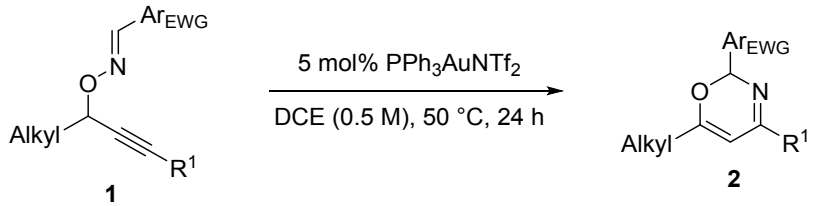
1t (Ar$_{EWG}$ = *p*-O$_2$NC$_6$H$_4$)

2t

To a solution of **1t** (67.3 mg, 0.2 mmol) and pyridine (1.6 μL, 0.02 mmol) in DCE (0.4 mL) in a V-vial under argon atmosphere was added PPh_3AuNTf_2 (7.4 mg, 0.01 mmol). The resulting mixture was stirred at 50 °C for 62 h, then passed through a short pad of silica gel with CH_2Cl_2 (50 mL). After removing the solvents *in vacuo*, the crude product was purified by silica gel flash column chromatography using hexane/EtOAc [5/1 (v/v)] as eluent to afford **2t** (0.18 mmol 60.6 mg, 90%) in an analytically pure form.

6. Au-catalyzed reaction of 1t-1y without pyridine

Table S2. Au-Catalyzed Reaction of 1t-1y without Pyridine.



1 (Ar$_{EWG}$ = *p*-O$_2$NC$_6$H$_4$)

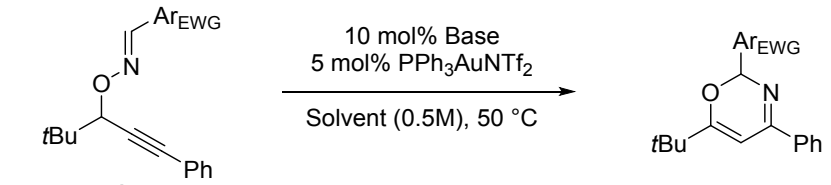
2

	1	R^1	Alkyl	**2** (%)[a]	**1** (%)[a]
1	1t	Ph	*t*Bu	<1	90
2	1u	Ph	*i*Pr	<1	86
3	1v	Ph	Cy	<1	83
4	1w	Ph	cyclopropyl	<1	85
5	1x	Ph	*n*Pr	<1	77
6	1y	Cy	*t*Bu	<1	80

[a] The yields were determined by ^{1}H NMR using dibromomethane as an internal standard.

7. Screening of Brønsted base catalyst

Table S3. Screening of Brønsted Base Catalyst.



1t (Ar$_{EWG}$ = *p*-O$_2$NC$_6$H$_4$)

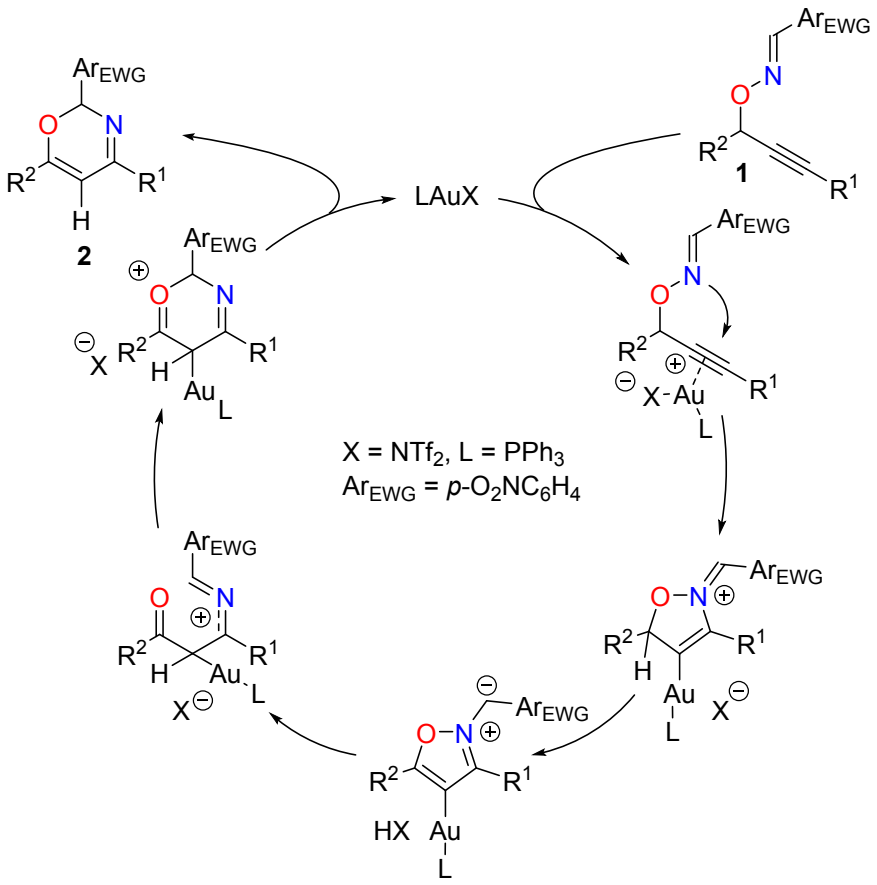
2t

	Base	Solvent	time (h)	**2t** (%)[a]	**1t** (%)[a]
1	none	DCE	8	<1	90
2	KO*t*Bu	DMSO	24	<1	75
3	NaOH	DMSO	24	<1	87
4	K_3PO_4	DMSO	24	<1	98
5	LiHMDS	DMSO	24	<1	83
6	TMG	DCE	24	<1	99
7	TBD	DCE	24	<1	95
8	DBU	DCE	24	<1	96
9	DABCO	DCE	24	5	89
10	piperidine	DCE	24	34	38
11	TEA	DCE	24	6	33
12	protone sponge	DCE	24	9	25
13	DMAP	DCE	24	17	78
14	2,2'-bipyridine	DCE	24	25	63
15	2,6-di-tert-butylpyridine	DCE	24	23	66
16	2,6-lutidine	DCE	24	10	64
17	pyridine	DCE	24	41	51
18	pyridine	DCE	62	(90)	<1

[a] The yields were determined by ^{1}H NMR using dibromomethane as an internal standard. Isolated yields in the parentheses.

8. A plausible catalytic cycle for Au-catalyzed reaction of 1 via N-O bond cleavage

Scheme S1. A proposed mechanism.



9. X-ray crystallographic analysis of 2s

Experimental

Data Collection

A colorless platelet crystal of $C_{26}H_{18}N_2O_3$ having approximate dimensions of 0.300 x 0.200 x 0.020 mm was mounted on a glass fiber. All measurements were made on a Rigaku XtaLAB mini diffractometer using graphite monochromated Mo-Kα radiation.

The crystal-to-detector distance was 50.00 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive orthorhombic cell with dimensions:

a = 22.596(3) Å
b = 3.8694(5) Å
c = 22.166(3) Å
V = 1938.0(4) $Å^3$

For Z = 4 and F.W. = 406.44, the calculated density is 1.393 g/cm^3. Based on the reflection conditions of:

0kl: k+l = 2n
h0l: h = 2n

packing considerations, a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

$Pna2_1$ (#33)

The data were collected at a temperature of -123 ± 1°C to a maximum 2θ value of 55.0°. A total of 540 oscillation images were collected. A sweep of data was done using ω scans from -60.0 to 120.0° in 1.00° step, at χ=54.0° and ϕ = 0.0°. The exposure rate was 32.0 [sec./°]. The detector swing angle was 30.00°. A second sweep was performed using ω scans from -60.0 to 120.0° in 1.00° step, at χ=54.0° and ϕ = 120.0°. The exposure rate was 32.0 [sec./°]. The detector swing angle was 30.00°. Another sweep was performed using ω scans from -60.0 to 120.0° in 1.00° step, at χ=54.0° and ϕ = 240.0°. The exposure rate was 32.0 [sec./°]. The detector swing

angle was 30.00°. Another sweep was performed using ω scans from -60.0 to 120.0° in 1.00° step, at χ=54.0° and ϕ = 0.0°. The exposure rate was 32.0 [sec./°]. The detector swing angle was 30.00°. Another sweep was performed using ω scans from -60.0 to 120.0° in 1.00° step, at χ=54.0° and ϕ = 120.0°. The exposure rate was 32.0 [sec./°]. The detector swing angle was 30.00°. Another sweep was performed using ω scans from -60.0 to 120.0° in 1.00° step, at χ=54.0° and ϕ = 240.0°. The exposure rate was 32.0 [sec./°]. The detector swing angle was 30.00°. The crystal-to-detector distance was 50.00 mm. Readout was performed in the 0.073 mm pixel mode.

Data Reduction

Of the 18117 reflections were collected, where 4389 were unique (R_{int} = 0.0350). Data were collected and processed using CrystalClear (Rigaku). [1]

The linear absorption coefficient, μ, for Mo-Kα radiation is 0.921 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.860 to 0.998. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[2] and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[3] on F^2 was based on 4389 observed reflections and 280 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0366$$

$$wR2 = [\Sigma (w (Fo^2 - Fc^2)^2) / \Sigma \, w(Fo^2)^2]^{1/2} = 0.0852$$

The goodness of fit[4] was 1.07. Unit weights were used. Plots of Σ w $(|Fo| - |Fc|)^2$ versus |Fo|, reflection order in data collection, sin θ/λ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.20 and -0.20 $e^-/Å^3$, respectively. The final Flack parameter [5] was 0.2(9), indicating that inversion-distinguishing power is too weak.[6] It is required to avarage Friedel pairs and do least-squares structure refinement again.

Neutral atom scattering factors were taken from International Tables for Crystallography (IT), Vol. C,

Table 6.1.1.4 [7]. Anomalous dispersion effects were included in Fcalc[8]; the values for Δf' and Δf'' were those of Creagh and McAuley[9]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[10]. All calculations were performed using the CrystalStructure[11] crystallographic software package except for refinement, which was performed using SHELXL97[12].

References

(1) CrystalClear: Data Collection and Processing Software, Rigaku Corporation (1998-2014). Tokyo 196-8666, Japan.

(2) SIR2008: Burla, M. C., Caliandro, R., Camalli, M., Carrozzini, B., Cascarano, G. L., De Caro, L., Giacovazzo, C., Polidori, G. Siliqi, D. and Spagna R. (2007). J. Appl. Cryst. 40, 609-613.

(3) Least Squares function minimized: (SHELXL97)

$\Sigma w(F_o^2-F_c^2)^2$ where w = Least Squares weights.

(4) Goodness of fit is defined as:

$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$

where: N_o = number of observations

N_v = number of variables

(5) Flack, H. D. (1983), Acta Cryst. A39, 876-881.

(6) Flack, H.D. and Bernardinelli (2000), J. Appl. Cryst. 33, 114-1148.

(7) International Tables for Crystallography, Vol.C (1992). Ed. A.J.C. Wilson, Kluwer Academic Publishers, Dordrecht, Netherlands, Table 6.1.1.4, pp. 572.

(8) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(9) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.),

Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(10) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(11) CrystalStructure 4.1: Crystal Structure Analysis Package, Rigaku Corporation (2000-2014). Tokyo 196-8666, Japan.

(12) SHELXL97: Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{26}H_{18}N_2O_3$
Formula Weight	406.44
Crystal Color, Habit	colorless, platelet
Crystal Dimensions	0.300 X 0.200 X 0.020 mm
Crystal System	orthorhombic
Lattice Type	Primitive
Lattice Parameters	a = 22.596(3) Å b = 3.8694(5) Å c = 22.166(3) Å V = 1938.0(4) Å^3
Space Group	$Pna2_1$ (#33)
Z value	4
D_{calc}	1.393 g/cm^3
F_{000}	848.00
μ(MoKα)	0.921 cm^{-1}

B. Intensity Measurements

Diffractometer	XtaLAB mini
Radiation	MoKα (λ = 0.71075 Å) graphite monochromated
Voltage, Current	50kV, 12mA
Temperature	-123.0°C
Detector Aperture	75.0 mm (diameter)
Data Images	540 exposures
ω oscillation Range (χ=54.0, ϕ=0.0)	-60.0 - 120.0°
Exposure Rate	32.0 sec./°
Detector Swing Angle	30.00°
ω oscillation Range (χ=54.0, ϕ=120.0)	-60.0 - 120.0°
Exposure Rate	32.0 sec./°
Detector Swing Angle	30.00°
ω oscillation Range (χ=54.0, ϕ=240.0)	-60.0 - 120.0°
Exposure Rate	32.0 sec./°
Detector Swing Angle	30.00°
ω oscillation Range (χ=54.0, ϕ=0.0)	-60.0 - 120.0°
Exposure Rate	32.0 sec./°

Detector Swing Angle	30.00°
ω oscillation Range (χ=54.0, ϕ=120.0)	-60.0 - 120.0°
Exposure Rate	32.0 sec./°
Detector Swing Angle	30.00°
ω oscillation Range (χ=54.0, ϕ=240.0)	-60.0 - 120.0°
Exposure Rate	32.0 sec./°
Detector Swing Angle	30.00°
Detector Position	50.00 mm
Pixel Size	0.073 mm
$2\theta_{max}$	55.0°
No. of Reflections Measured	Total: 18117 Unique: 4389 (R_{int} = 0.0350) Friedel pairs: 2133
Corrections	Lorentz-polarization Absorption (trans. factors: 0.860 - 0.998)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR2008)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w $(Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/ [\sigma^2(Fo^2) + (0.0420 \cdot P)^2 + 0.2923 \cdot P]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	55.0^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	4389
No. Variables	280
Reflection/Parameter Ratio	15.68
Residuals: R1 (I>2.00σ(I))	0.0366
Residuals: R (All reflections)	0.0411
Residuals: wR2 (All reflections)	0.0852
Goodness of Fit Indicator	1.072
Flack Parameter (Friedel pairs = 2133)	0.2(9)
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	0.20 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.20 $e^-/Å^3$

Table S4. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
O1	0.47939(4)	0.5299(3)	0.66264(5)	1.360(17)
O2	0.57917(6)	1.0040(4)	0.38903(6)	3.37(3)
O9	0.66821(6)	1.0484(5)	0.42325(7)	3.69(3)
N16	0.61629(7)	0.9621(4)	0.42853(6)	2.10(3)
N30	0.57784(6)	0.4731(3)	0.70401(6)	1.44(2)
C2	0.38979(7)	0.4433(4)	0.71666(7)	1.41(2)
C3	0.58993(7)	0.4585(4)	0.81147(7)	1.46(2)
C4	0.29257(7)	0.4113(4)	0.66793(7)	1.70(3)
C5	0.45498(7)	0.4180(4)	0.71536(7)	1.35(2)
C6	0.35428(7)	0.3391(4)	0.66594(7)	1.45(2)
C7	0.55973(7)	0.5412(4)	0.59458(6)	1.35(2)
C8	0.55324(7)	0.4196(4)	0.75585(7)	1.41(2)
C10	0.52025(7)	0.5733(5)	0.54651(7)	1.73(3)
C11	0.26778(7)	0.5708(5)	0.71969(8)	2.03(3)
C12	0.36332(7)	0.5868(4)	0.76663(7)	1.77(3)
C13	0.64936(7)	0.3634(5)	0.81047(8)	1.79(3)
C14	0.61826(7)	0.6411(4)	0.58711(7)	1.57(3)
C15	0.34102(8)	0.0736(5)	0.56758(7)	1.94(3)
C17	0.65913(8)	0.5163(5)	0.91508(8)	2.07(3)
C18	0.37697(7)	0.1593(4)	0.61514(7)	1.56(3)
C19	0.63753(7)	0.7756(4)	0.53218(7)	1.68(3)
C20	0.68364(8)	0.3887(5)	0.86213(8)	2.01(3)
C21	0.60030(8)	0.6159(5)	0.91629(7)	2.01(3)
C22	0.59689(7)	0.8077(4)	0.48592(7)	1.55(3)
C23	0.53875(6)	0.3937(4)	0.65419(7)	1.38(2)
C24	0.25691(7)	0.3190(5)	0.61765(8)	2.14(3)
C25	0.30192(8)	0.6477(5)	0.76863(8)	2.12(3)
C26	0.53853(7)	0.7081(5)	0.49170(7)	1.79(3)
C27	0.28056(8)	0.1581(5)	0.56873(8)	2.24(3)
C28	0.49064(7)	0.3347(4)	0.76188(7)	1.54(3)
C29	0.56533(7)	0.5837(4)	0.86489(8)	1.78(3)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table S5. Atomic coordinates and B_{iso} involving hydrogen atoms

atom	x	y	z	B_{iso}
H10	0.48032	0.50169	0.55142	2.077
H11	0.22677	0.62488	0.72029	2.435
H12	0.38698	0.64607	0.80051	2.120
H13	0.66653	0.28058	0.77412	2.148
H14	0.64535	0.61761	0.61963	1.881
H15	0.35710	-0.04353	0.53367	2.333
H17	0.68269	0.53515	0.95042	2.482
H18	0.41765	0.09752	0.61407	1.876
H19	0.67757	0.84340	0.52668	2.021
H20	0.72393	0.31871	0.86131	2.414
H21	0.58372	0.70671	0.95234	2.411
H23	0.53607	0.13677	0.65019	1.655
H24	0.21581	0.37053	0.61823	2.573
H25	0.28434	0.74189	0.80392	2.542
H26	0.51164	0.73141	0.45901	2.152
H27	0.25613	0.10261	0.53522	2.682
H28	0.47564	0.22530	0.79707	1.851
H29	0.52472	0.64687	0.86620	2.137

Table S6. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O1	0.0148(5)	0.0205(5)	0.0164(5)	-0.0004(4)	0.0006(4)	0.0014(4)
O2	0.0423(9)	0.0648(10)	0.0210(6)	-0.0123(7)	-0.0048(6)	0.0144(7)
O9	0.0319(8)	0.0760(11)	0.0323(7)	-0.0138(7)	0.0066(6)	0.0162(8)
N16	0.0294(8)	0.0323(8)	0.0181(7)	-0.0035(6)	0.0042(6)	0.0018(6)
N30	0.0192(6)	0.0201(7)	0.0153(6)	0.0023(5)	0.0001(5)	-0.0007(5)
C2	0.0188(8)	0.0150(7)	0.0199(8)	-0.0013(6)	0.0014(6)	0.0033(6)
C3	0.0205(8)	0.0197(8)	0.0154(7)	-0.0021(6)	-0.0008(6)	0.0026(6)
C4	0.0187(8)	0.0192(8)	0.0266(8)	-0.0027(6)	-0.0003(7)	0.0085(7)
C5	0.0184(7)	0.0146(7)	0.0182(7)	-0.0033(6)	0.0015(6)	-0.0017(6)
C6	0.0180(7)	0.0162(7)	0.0208(7)	-0.0033(6)	0.0008(6)	0.0067(6)
C7	0.0211(8)	0.0153(7)	0.0148(7)	0.0019(6)	0.0013(6)	-0.0039(6)
C8	0.0192(8)	0.0154(7)	0.0189(7)	0.0019(6)	-0.0007(6)	-0.0010(6)
C10	0.0194(8)	0.0276(9)	0.0188(8)	-0.0056(7)	0.0006(6)	-0.0009(7)
C11	0.0175(8)	0.0240(8)	0.0355(10)	0.0010(7)	0.0071(7)	0.0078(7)
C12	0.0240(8)	0.0230(8)	0.0202(8)	-0.0031(7)	0.0021(7)	-0.0007(7)
C13	0.0221(8)	0.0250(9)	0.0209(8)	0.0001(6)	0.0011(7)	0.0021(7)
C14	0.0191(8)	0.0228(8)	0.0176(7)	0.0026(6)	-0.0010(6)	-0.0002(6)
C15	0.0315(9)	0.0218(8)	0.0205(8)	-0.0065(7)	-0.0017(7)	0.0035(7)
C17	0.0296(9)	0.0299(9)	0.0191(8)	-0.0073(7)	-0.0061(7)	0.0059(7)
C18	0.0203(8)	0.0186(8)	0.0204(8)	-0.0032(6)	0.0003(6)	0.0041(6)
C19	0.0173(7)	0.0254(8)	0.0213(8)	0.0009(6)	0.0025(6)	0.0001(7)
C20	0.0207(8)	0.0299(10)	0.0258(9)	-0.0015(7)	-0.0026(7)	0.0062(7)
C21	0.0306(9)	0.0306(9)	0.0152(8)	-0.0072(7)	0.0020(7)	-0.0027(7)
C22	0.0238(8)	0.0201(8)	0.0151(7)	-0.0001(6)	0.0033(6)	-0.0003(6)
C23	0.0176(7)	0.0172(8)	0.0176(7)	0.0020(6)	0.0004(6)	-0.0008(6)
C24	0.0182(8)	0.0273(9)	0.0360(9)	-0.0033(7)	-0.0068(7)	0.0102(8)
C25	0.0272(9)	0.0243(9)	0.0290(9)	0.0021(7)	0.0129(7)	0.0022(7)
C26	0.0235(8)	0.0292(9)	0.0155(7)	-0.0020(7)	-0.0040(6)	-0.0021(7)
C27	0.0305(9)	0.0281(10)	0.0263(9)	-0.0107(7)	-0.0120(7)	0.0066(7)
C28	0.0212(8)	0.0217(8)	0.0157(7)	-0.0023(6)	0.0032(6)	0.0011(6)
C29	0.0199(8)	0.0259(9)	0.0219(8)	-0.0008(7)	0.0018(7)	-0.0011(7)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table S7. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
O1	C5	1.3627(19)	O1	C23	1.4532(17)
O2	N16	1.223(2)	O9	N16	1.225(2)
N16	C22	1.472(2)	N30	C8	1.293(2)
N30	C23	1.447(2)	C2	C5	1.477(2)
C2	C6	1.439(2)	C2	C12	1.376(2)
C3	C8	1.493(2)	C3	C13	1.393(2)
C3	C29	1.395(2)	C4	C6	1.423(2)
C4	C11	1.418(2)	C4	C24	1.421(2)
C5	C28	1.348(2)	C6	C18	1.419(2)
C7	C10	1.395(2)	C7	C14	1.388(2)
C7	C23	1.515(2)	C8	C28	1.458(2)
C10	C26	1.385(2)	C11	C25	1.364(2)
C12	C25	1.408(2)	C13	C20	1.386(2)
C14	C19	1.394(2)	C15	C18	1.372(2)
C15	C27	1.405(3)	C17	C20	1.389(3)
C17	C21	1.384(3)	C19	C22	1.382(2)
C21	C29	1.392(2)	C22	C26	1.380(2)
C24	C27	1.360(3)			

Table S8. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C10	H10	0.950	C11	H11	0.950
C12	H12	0.950	C13	H13	0.950
C14	H14	0.950	C15	H15	0.950
C17	H17	0.950	C18	H18	0.950
C19	H19	0.950	C20	H20	0.950
C21	H21	0.950	C23	H23	1.000
C24	H24	0.950	C25	H25	0.950
C26	H26	0.950	C27	H27	0.950
C28	H28	0.950	C29	H29	0.950

Table S9. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
C5	O1	C23	111.65(11)	O2	N16	O9	123.50(15)
O2	N16	C22	117.91(15)	O9	N16	C22	118.57(14)
C8	N30	C23	112.44(13)	C5	C2	C6	121.50(14)
C5	C2	C12	118.43(14)	C6	C2	C12	119.98(14)
C8	C3	C13	119.71(14)	C8	C3	C29	120.97(14)
C13	C3	C29	119.31(15)	C6	C4	C11	119.85(14)
C6	C4	C24	118.81(14)	C11	C4	C24	121.33(15)
O1	C5	C2	113.55(13)	O1	C5	C28	119.35(14)
C2	C5	C28	126.68(14)	C2	C6	C4	117.85(14)
C2	C6	C18	123.76(14)	C4	C6	C18	118.35(14)
C10	C7	C14	119.57(13)	C10	C7	C23	119.96(14)
C14	C7	C23	120.47(13)	N30	C8	C3	118.61(14)
N30	C8	C28	122.31(14)	C3	C8	C28	119.05(14)
C7	C10	C26	120.84(15)	C4	C11	C25	121.00(15)
C2	C12	C25	121.42(15)	C3	C13	C20	120.47(16)
C7	C14	C19	120.39(14)	C18	C15	C27	120.38(15)
C20	C17	C21	119.89(16)	C6	C18	C15	120.95(15)
C14	C19	C22	118.30(15)	C13	C20	C17	120.04(16)
C17	C21	C29	120.28(15)	N16	C22	C19	118.67(14)
N16	C22	C26	118.56(14)	C19	C22	C26	122.75(15)
O1	C23	N30	112.83(12)	O1	C23	C7	105.35(12)
N30	C23	C7	113.24(12)	C4	C24	C27	121.18(15)
C11	C25	C12	119.72(16)	C10	C26	C22	118.14(14)
C15	C27	C24	120.21(16)	C5	C28	C8	117.12(14)
C3	C29	C21	119.98(15)				

Table S10. Bond angles involving hydrogens (^{O})

atom	atom	atom	angle	atom	atom	atom	angle
C7	C10	H10	119.6	C26	C10	H10	119.6
C4	C11	H11	119.5	C25	C11	H11	119.5
C2	C12	H12	119.3	C25	C12	H12	119.3
C3	C13	H13	119.8	C20	C13	H13	119.8
C7	C14	H14	119.8	C19	C14	H14	119.8
C18	C15	H15	119.8	C27	C15	H15	119.8
C20	C17	H17	120.1	C21	C17	H17	120.0
C6	C18	H18	119.5	C15	C18	H18	119.5
C14	C19	H19	120.9	C22	C19	H19	120.8
C13	C20	H20	120.0	C17	C20	H20	120.0
C17	C21	H21	119.9	C29	C21	H21	119.9
O1	C23	H23	108.4	N30	C23	H23	108.4
C7	C23	H23	108.4	C4	C24	H24	119.4
C27	C24	H24	119.4	C11	C25	H25	120.1
C12	C25	H25	120.1	C10	C26	H26	120.9
C22	C26	H26	120.9	C15	C27	H27	119.9
C24	C27	H27	119.9	C5	C28	H28	121.4
C8	C28	H28	121.4	C3	C29	H29	120.0
C21	C29	H29	120.0				

Table S11. Torsion Angles(°)

(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C5	O1	C23	N30	-55.67(15)	C5	O1	C23	C7	-179.68(10)
C23	O1	C5	C2	-159.85(10)	C23	O1	C5	C28	27.16(17)
O2	N16	C22	C19	-176.58(14)	O2	N16	C22	C26	2.0(2)
O9	N16	C22	C19	1.9(2)	O9	N16	C22	C26	-179.52(14)
C8	N30	C23	O1	45.10(17)	C8	N30	C23	C7	164.66(12)
C23	N30	C8	C3	174.38(11)	C23	N30	C8	C28	-7.8(2)
C5	C2	C6	C4	-172.36(12)	C5	C2	C6	C18	9.7(2)
C6	C2	C5	O1	43.80(19)	C6	C2	C5	C28	-143.82(14)
C5	C2	C12	C25	174.15(12)	C12	C2	C5	O1	-132.82(14)
C12	C2	C5	C28	39.6(2)	C6	C2	C12	C25	-2.5(2)
C12	C2	C6	C4	4.2(2)	C12	C2	C6	C18	-173.72(13)
C8	C3	C13	C20	-178.19(13)	C13	C3	C8	N30	-35.1(2)
C13	C3	C8	C28	146.98(14)	C8	C3	C29	C21	179.64(13)
C29	C3	C8	N30	145.93(15)	C29	C3	C8	C28	-32.0(2)
C13	C3	C29	C21	0.7(2)	C29	C3	C13	C20	0.8(2)
C6	C4	C11	C25	-1.9(2)	C11	C4	C6	C2	-2.0(2)
C11	C4	C6	C18	176.00(13)	C6	C4	C24	C27	1.3(2)
C24	C4	C6	C2	178.35(13)	C24	C4	C6	C18	-3.6(2)
C11	C4	C24	C27	-178.29(14)	C24	C4	C11	C25	177.67(14)
O1	C5	C28	C8	9.1(2)	C2	C5	C28	C8	-162.89(13)
C2	C6	C18	C15	-178.59(13)	C4	C6	C18	C15	3.5(2)
C10	C7	C14	C19	0.6(2)	C14	C7	C10	C26	-0.9(2)
C10	C7	C23	O1	-38.24(18)	C10	C7	C23	N30	-162.01(13)
C23	C7	C10	C26	179.85(13)	C14	C7	C23	O1	142.55(13)
C14	C7	C23	N30	18.79(19)	C23	C7	C14	C19	179.78(12)
N30	C8	C28	C5	-20.5(2)	C3	C8	C28	C5	157.35(13)
C7	C10	C26	C22	0.4(2)	C4	C11	C25	C12	3.7(2)
C2	C12	C25	C11	-1.5(2)	C3	C13	C20	C17	-1.3(3)
C7	C14	C19	C22	0.3(2)	C18	C15	C27	C24	-1.4(3)
C27	C15	C18	C6	-1.0(2)	C20	C17	C21	C29	1.0(3)
C21	C17	C20	C13	0.4(3)	C14	C19	C22	N16	177.65(13)
C14	C19	C22	C26	-0.9(2)	C17	C21	C29	C3	-1.6(2)
N16	C22	C26	C10	-177.99(13)	C19	C22	C26	C10	0.6(2)
C4	C24	C27	C15	1.3(3)					

Table S12. Intramolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
O1	C6	2.9227(19)	O1	C8	2.6899(19)
O1	C10	2.7399(19)	O1	C12	3.4986(19)
O1	C14	3.5825(19)	O1	C18	2.9189(19)
O2	C19	3.548(2)	O2	C26	2.708(2)
O9	C19	2.725(2)	O9	C26	3.553(2)
N30	C5	2.796(2)	N30	C13	2.891(2)
N30	C14	2.823(2)	C2	C11	2.802(2)
C3	C17	2.787(2)	C4	C12	2.793(2)
C4	C15	2.802(2)	C5	C18	3.007(2)
C6	C25	2.830(2)	C6	C27	2.812(2)
C7	C22	2.751(2)	C10	C19	2.781(2)
C12	C28	3.040(2)	C13	C21	2.772(2)
C14	C26	2.790(2)	C18	C24	2.783(2)
C20	C29	2.778(2)	C23	C28	2.633(2)
C28	C29	2.998(2)			

Table S13. Intramolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
O1	H10	2.468	O1	H18	2.430
O1	H28	3.205	O2	H26	2.418
O9	H19	2.435	N16	H19	2.619
N16	H26	2.616	N30	H13	2.643
N30	H14	2.477	N30	H28	3.242
C2	H18	2.712	C2	H25	3.279
C2	H28	2.766	C3	H20	3.268
C3	H21	3.270	C3	H28	2.754
C4	H18	3.300	C4	H25	3.280
C4	H27	3.280	C5	H12	2.589
C5	H18	2.700	C5	H23	2.575
C6	H11	3.313	C6	H12	3.295
C6	H15	3.285	C6	H24	3.305
C7	H19	3.275	C7	H26	3.279
C8	H13	2.647	C8	H23	2.614
C8	H29	2.678	C10	H14	3.263
C10	H18	3.318	C10	H23	2.874
C11	H12	3.248	C11	H24	2.653
C12	H11	3.255	C12	H28	2.975
C13	H17	3.261	C13	H29	3.265
C14	H10	3.261	C14	H23	3.035
C15	H10	3.575	C15	H24	3.253
C17	H13	3.259	C17	H29	3.264
C18	H10	3.034	C18	H27	3.262
C19	H26	3.279	C20	H21	3.257
C21	H20	3.258	C22	H10	3.232
C22	H14	3.244	C23	H10	2.666
C23	H14	2.672	C23	H18	3.097
C23	H28	3.534	C24	H11	2.654
C24	H15	3.249	C26	H19	3.278
C27	H18	3.265	C28	H12	2.770
C28	H23	2.787	C28	H29	2.720
C29	H13	3.264	C29	H17	3.265
C29	H28	2.879	H10	H15	3.515
H10	H18	2.526	H10	H23	2.894

Table S13. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H10	H26	2.342	H11	H24	2.479
H11	H25	2.309	H12	H25	2.350
H12	H28	2.583	H12	H29	3.436
H13	H20	2.332	H14	H19	2.353
H14	H23	3.165	H15	H18	2.312
H15	H27	2.351	H17	H20	2.339
H17	H21	2.333	H18	H23	2.797
H21	H29	2.340	H23	H28	3.547
H24	H27	2.300	H28	H29	2.498

Table S14. Intermolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
O1	C18[1]	3.5210(19)	O2	C12[2]	3.400(2)
O2	C28[3]	3.485(2)	N16	C22[1]	3.538(2)
C2	C12[4]	3.545(2)	C2	C18[1]	3.581(2)
C4	C11[4]	3.494(2)	C4	C15[1]	3.566(2)
C6	C15[1]	3.595(2)	C6	C18[1]	3.407(2)
C7	C23[1]	3.585(2)	C10	C26[4]	3.585(2)
C11	C4[1]	3.494(2)	C12	O2[5]	3.400(2)
C12	C2[1]	3.545(2)	C14	C19[4]	3.590(2)
C15	C4[4]	3.566(2)	C15	C6[4]	3.595(2)
C18	O1[4]	3.5210(19)	C18	C2[4]	3.581(2)
C18	C6[4]	3.407(2)	C19	C14[1]	3.590(2)
C22	N16[4]	3.538(2)	C23	C7[4]	3.585(2)
C24	C27[1]	3.465(3)	C26	C10[1]	3.585(2)
C27	C24[4]	3.465(3)	C28	O2[6]	3.485(2)

Symmetry Operators:

(1) X,Y+1,Z

(2) -X+1,-Y+2,Z+1/2-1

(3) -X+1,-Y+1,Z+1/2-1

(4) X,Y-1,Z

(5) -X+1,-Y+2,Z+1/2

(6) -X+1,-Y+1,Z+1/2

Table S15. Intermolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
O1	H18[1]	2.816	O1	H23[1]	2.689
O2	H12[2]	3.280	O2	H12[3]	2.504
O2	H26[1]	3.558	O2	H28[2]	2.545
O2	H29[2]	3.480	O2	H29[3]	2.755
O9	H12[3]	3.218	O9	H17[4]	3.423
O9	H20[4]	2.935	O9	H25[3]	2.967
O9	H27[5]	3.454	N16	H12[3]	3.218
N30	H23[1]	2.985	C2	H18[1]	3.461
C4	H11[6]	3.580	C5	H18[1]	3.559
C6	H18[1]	3.462	C7	H23[1]	2.668
C10	H18[1]	3.425	C10	H21[2]	3.324
C10	H23[1]	3.188	C11	H13[7]	2.922
C13	H11[8]	3.260	C13	H11[5]	3.313
C13	H25[5]	3.414	C14	H23[1]	3.014
C14	H24[8]	3.042	C14	H24[5]	2.984
C14	H27[8]	3.452	C15	H15[1]	3.517
C15	H17[9]	3.547	C15	H17[2]	3.053
C15	H21[2]	3.184	C17	H15[10]	3.223
C17	H15[11]	3.348	C17	H27[11]	3.596
C19	H24[5]	2.940	C19	H27[8]	3.054
C20	H25[8]	3.577	C20	H25[5]	2.981
C21	H10[11]	3.535	C21	H15[10]	3.550
C21	H15[11]	3.230	C21	H26[11]	3.017
C23	H23[1]	2.877	C24	H11[6]	3.585
C24	H14[7]	3.035	C24	H14[12]	3.333
C24	H19[12]	2.998	C24	H27[1]	3.540
C25	H13[7]	3.481	C25	H20[7]	3.253
C25	H20[12]	3.404	C26	H10[1]	3.593
C26	H21[2]	3.312	C26	H29[2]	3.416
C27	H14[7]	3.427	C27	H17[2]	2.996
C27	H19[7]	3.170	C27	H19[12]	3.163
C27	H24[6]	3.554	C28	H28[1]	3.550
C29	H26[11]	2.977	C29	H28[1]	3.540
H10	C21[2]	3.535	H10	C26[6]	3.593
H10	H15[1]	3.317	H10	H18[1]	3.041

Table S15. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

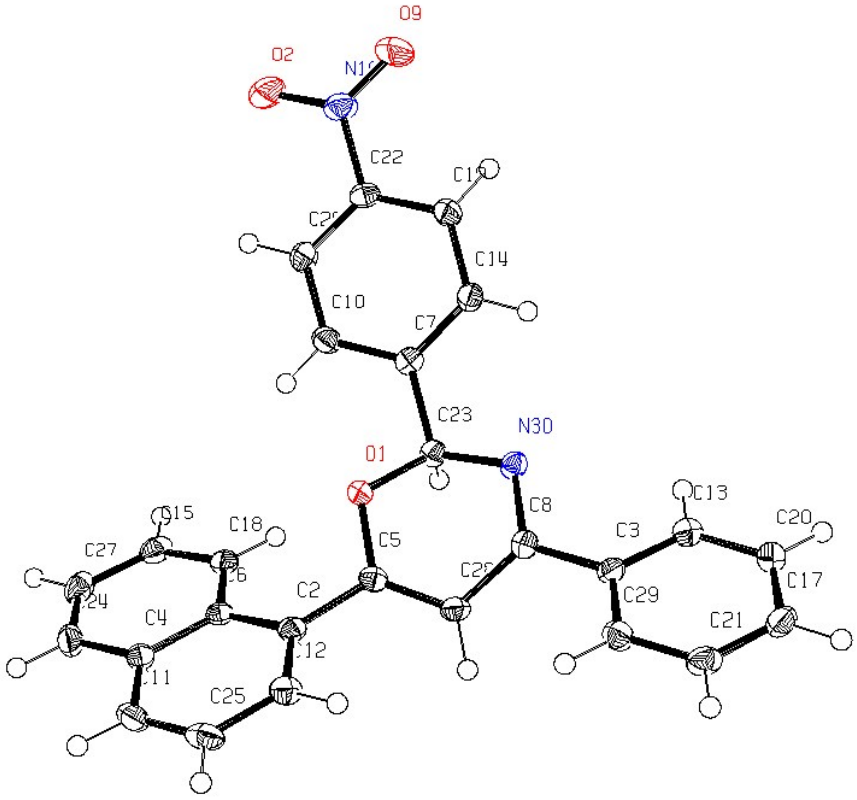
atom	atom	distance	atom	atom	distance
H10	H21[2]	2.751	H10	H23[1]	3.524
H11	C4[1]	3.580	H11	C13[7]	3.260
H11	C13[12]	3.313	H11	C24[1]	3.585
H11	H13[7]	2.395	H11	H13[12]	2.927
H11	H14[12]	3.059	H11	H20[7]	3.567
H12	O2[11]	3.280	H12	O2[13]	2.504
H12	O9[13]	3.218	H12	N16[13]	3.218
H12	H28[1]	3.007	H13	C11[8]	2.922
H13	C25[8]	3.481	H13	H11[8]	2.395
H13	H11[5]	2.927	H13	H25[8]	3.407
H13	H25[5]	3.307	H14	C24[8]	3.035
H14	C24[5]	3.333	H14	C27[8]	3.427
H14	H11[5]	3.059	H14	H23[1]	3.254
H14	H24[8]	2.471	H14	H24[5]	2.541
H14	H27[8]	3.239	H15	C15[6]	3.517
H15	C17[9]	3.223	H15	C17[2]	3.348
H15	C21[9]	3.550	H15	C21[2]	3.230
H15	H10[6]	3.317	H15	H17[9]	2.799
H15	H17[2]	2.843	H15	H21[9]	3.409
H15	H21[2]	2.596	H17	O9[14]	3.423
H17	C15[10]	3.547	H17	C15[11]	3.053
H17	C27[11]	2.996	H17	H15[10]	2.799
H17	H15[11]	2.843	H17	H27[10]	3.396
H17	H27[11]	2.722	H18	O1[6]	2.816
H18	C2[6]	3.461	H18	C5[6]	3.559
H18	C6[6]	3.462	H18	C10[6]	3.425
H18	H10[6]	3.041	H19	C24[5]	2.998
H19	C27[8]	3.170	H19	C27[5]	3.163
H19	H24[8]	3.535	H19	H24[5]	2.468
H19	H27[8]	2.483	H19	H27[5]	2.790
H20	O9[14]	2.935	H20	C25[8]	3.253
H20	C25[5]	3.404	H20	H11[8]	3.567
H20	H25[8]	2.861	H20	H25[5]	2.524
H21	C10[11]	3.324	H21	C15[11]	3.184
H21	C26[11]	3.312	H21	H10[11]	2.751

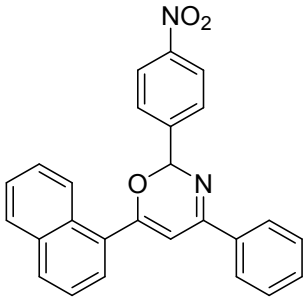
Table S15. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H21	H15[10]	3.409	H21	H15[11]	2.596
H21	H26[11]	2.746	H21	H26[13]	3.065
H23	O1[6]	2.689	H23	N30[6]	2.985
H23	C7[6]	2.668	H23	C10[6]	3.188
H23	C14[6]	3.014	H23	C23[6]	2.877
H23	H10[6]	3.524	H23	H14[6]	3.254
H24	C14[7]	3.042	H24	C14[12]	2.984
H24	C19[12]	2.940	H24	C27[1]	3.554
H24	H14[7]	2.471	H24	H14[12]	2.541
H24	H19[7]	3.535	H24	H19[12]	2.468
H24	H27[1]	3.499	H25	O9[13]	2.967
H25	C13[12]	3.414	H25	C20[7]	3.577
H25	C20[12]	2.981	H25	H13[7]	3.407
H25	H13[12]	3.307	H25	H20[7]	2.861
H25	H20[12]	2.524	H26	O2[6]	3.558
H26	C21[2]	3.017	H26	C29[2]	2.977
H26	H21[2]	2.746	H26	H21[3]	3.065
H26	H29[2]	2.655	H26	H29[3]	3.270
H27	O9[12]	3.454	H27	C14[7]	3.452
H27	C17[2]	3.596	H27	C19[7]	3.054
H27	C24[6]	3.540	H27	H14[7]	3.239
H27	H17[9]	3.396	H27	H17[2]	2.722
H27	H19[7]	2.483	H27	H19[12]	2.790
H27	H24[6]	3.499	H28	O2[11]	2.545
H28	C28[6]	3.550	H28	C29[6]	3.540
H28	H12[6]	3.007	H28	H29[6]	2.930
H29	O2[11]	3.480	H29	O2[13]	2.755
H29	C26[11]	3.416	H29	H26[11]	2.655
H29	H26[13]	3.270	H29	H28[1]	2.930

Symmetry Operators:

(1) X,Y+1,Z
(2) -X+1,-Y+1,Z+1/2-1
(3) -X+1,-Y+2,Z+1/2-1
(4) -X+1/2+1,Y+1/2,Z+1/2-1
(5) X+1/2,-Y+1/2+1,Z
(6) X,Y-1,Z
(7) X+1/2-1,-Y+1/2,Z
(8) X+1/2,-Y+1/2,Z
(9) -X+1,-Y,Z+1/2-1
(10) -X+1,-Y,Z+1/2
(11) -X+1,-Y+1,Z+1/2
(12) X+1/2-1,-Y+1/2+1,Z
(13) -X+1,-Y+2,Z+1/2
(14) -X+1/2+1,Y+1/2-1,Z+1/2

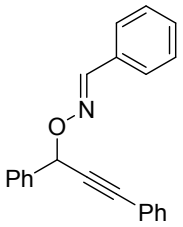




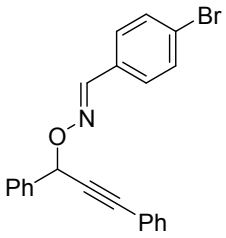
2q

Figure S3. X-ray crystallographic analysis of 2s in 50% ellipsoid probability

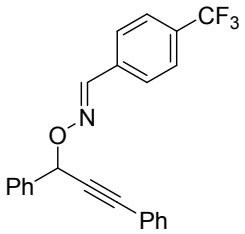
10. Analytical data of 1



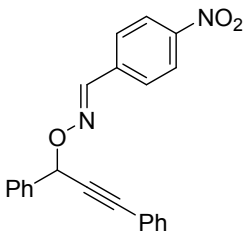
(*E*)-benzaldehyde *O*-(1,3-diphenylprop-2-yn-1-yl) oxime (1a). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.18 (s, 1H), 7.28-7.31 (m, 3H), 7.35-7.46 (m, 6H), 7.49-7.52 (m, 2H), 7.59-7.61 (m, 2H), 7.67-7.69 (m, 2H), 8.17 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 76.19, 86.75, 87.76, 122.49, 127.26, 128.07, 128.19, 128.52, 128.62, 128.74, 129.98, 131.56, 131.95, 137.74, 149.79. IR (neat) 3061, 3030, 2894, 2229, 1953, 1881, 1808, 1755, 1671,1598, 1572, 1489, 1445, 1302, 1276, 1210, 1016, 997, 970, 932 cm-1. HRMS (ESI) calcd. for $(M+Na)^+$ 334.12020869, found 334.1200.



(*E*)-4-bromobenzaldehyde *O*-(1,3-diphenylprop-2-yn-1-yl) oxime (1b). Colorless solid. Mp: 103.7 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.16 (s, 1H), 7.30-7.32 m, 3H), 7.35-7.50 (m, 9H), 7.66 (d, *J* = 7.3 Hz, 2H), 8.10 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 76.39, 86.56, 87.90, 122.40, 124.20, 128.08, 128.23, 128.55, 128.61, 128.66, 128.83, 130.91, 131.87, 137.55, 148.68. IR (neat) 362, 3033, 2897, 2229, 190, 1489, 1455, 1230, 1279, 1069, 1011, 938, 820, 756 cm^{-1}. HRMS (ESI) calcd. for $(M+Na)^+$ 414.0287, found 414.0287.

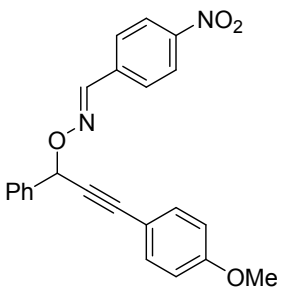


(*E*)-4-(trifluoromethyl)benzaldehyde *O*-(1,3-diphenylprop-2-yn-1-yl) oxime (1c). Colorless solid. Mp: 71.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.20 (s, 1H), 7.30-7.32 (m, 3H), 7.36-7.45 (m, 3H), 7.49-7.52 (m, 2H), 7.61 (d, *J* = 8.2 Hz, 2H), 7.67-7.72 (m, 4H), 8.18 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 76.65, 86.40, 88.06, 123.88 (q, *J* = 272.2 Hz), 125.60 (q, *J* = 3.8 Hz), 127.43, 128.12, 128.26, 128.60, 128.68, 128.92, 131.58 (q, *J* = 32.6 Hz), 131.88, 135.42, 137.43. IR (neat) 3064, 303 , 2897, 2230, 1324, 1168, 1126, 1066, 945, 795 cm^{-1}. HRMS (ESI) calcd. for $(M+Na)^+$ 402.1076, found 402.1076.

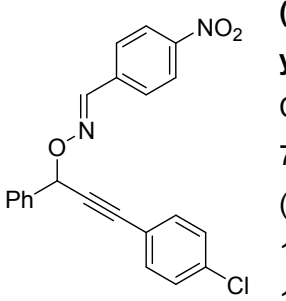


(*E*)-4-nitrobenzaldehyde *O*-(1,3-diphenylprop-2-yn-1-yl) oxime (1d). Yellow solid. Mp: 118.6 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.21 (s, 1H), 7.29-7.33 (m,3H), 7.38-7.46 (m, 3H), 7.50-7.51 (m, 2H), 7.67 (d, *J* = 6.9 Hz, 2H), 7.76 (d, *J* = 8.7 Hz, 2H), 8.20-8.23 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 77.09, 86.32, 88.38, 122.44, 123.95, 127.86, 128.12, 128.31, 128.62, 128.76, 128.97, 131.90, 137.43,

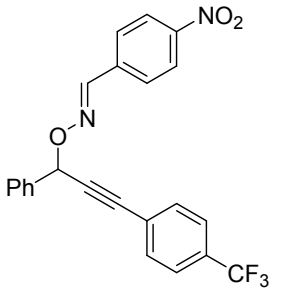
138.20, 147.53, 148.65. IR (neat) 3117, 3061, 2928, 2852, 1628, 1575, 1519, 1492, 1450, 1346, 1097, 1060, 8520 cm^{-1}. HRMS (ESI) calcd. for $(M+Na)^+$ 294.1101, found 294.1100.



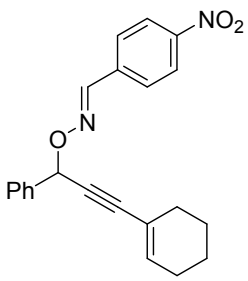
(*E*)-4-nitrobenzaldehyde *O*-(3-(4-methoxyphenyl)-1-phenylprop-2-yn-1-yl) oxime (1e). Yellow solid. Mp: 103.5 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 3.80 (s, 3H), 6.20 (s, 1H), 6.84 (d, *J* = 8.7 Hz, 2H), 7.38-7.46 (m, 5H), 7.67 (d, *J* = 6.9 Hz, 2H), 7.75 (d, *J* = 8.7 Hz, 2H), 8.20-8.26 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 55. 26, 77.09, 84.75, 88.29, 113.87, 114.23, 123.93, 127.81, 128.11, 128.59, 128.94, 133.38, 137.40, 138.12, 147.43, 148.35, 159.89. IR (neat) 3065, 3033, 2936, 2838, 2227, 1605, 1509, 1455, 1343, 1291, 1249, 1173, 1249, 1173, 1107, 1032, 948, 835 cm^{-1}. HRMS (ESI) calcd. for $(M+Na)^+$ 409.1159, found 409.1159.



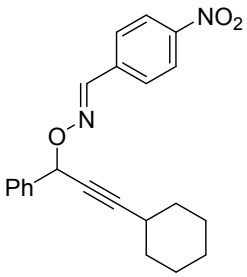
(*E*)-4-nitrobenzaldehyde *O*-(3-(4-chlorophenyl)-1-phenylprop-2-yn-1-yl) oxime (1f). Yellow solid. Mp: 124.8 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 6.19 (s, 1H), 7.27-7.30 (m, 2H), 7.40-7.46 (m, 5H), 7.64-7.67 (m, 2H), 7.75 (d, *J* = 8.7 Hz, 2H), 8.19-8.22 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 76.83, 87.03, 87.15, 120.65, 123.92, 127.81, 128.05, 128.62, 128.66, 129.09, 133.07, 134.80, 136.94, 137.94, 147.61, 148.39. IR (neat) 3089, 3064, 3033, 2903, 2852, 2230, 1589, 1518, 1488, 1455, 1397, 1341, 1296, 1278, 1091, 1015, 943, 851, 830 cm^{-1}. HRMS (ESI) calcd. for $(M+Na)^+$ 413.0663, found 413.0663.



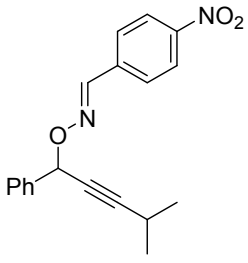
(*E*)-4-nitrobenzaldehyde *O*-(1-phenyl-3-(4-(trifluoromethyl)phenyl)prop-2-yn-1-yl) oxime (1g). Yellow solid. Mp: 90.7 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 6.22 (s, 1H), 7.39-7.47 (m, 3H), 7.59 (dd, *J* = 13.3, 8.7 Hz, 4H), 7.66 (d, *J* = 6.9 Hz, 2H), 7.76 (d, *J* = 8.7 Hz, 2H), 8.21-8.23 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 76.72, 86.69, 88.71, 123.75 (q. *J* = 272.2 Hz), 123.92, 125.19, 126.02, 127.82, 128.05, 128.70, 129.16, 130.39 (q, *J* = 32.6 Hz), 132.07, 136.75, 137.87, 147.72, 148.44. IR (neat) 3117, 3066, 3035, 2917, 2851, 1589, 1519, 1343, 1320, 1165, 1124, 1105, 1067, 1017, 940, 836 cm^{-1}. HRMS (ESI) calcd. for $(M+Na)^+$ 447.0927, found 447.0926.



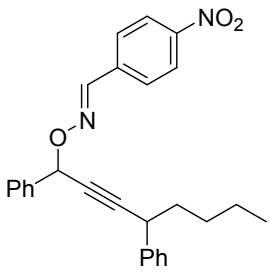
(*E*)-4-nitrobenzaldehyde *O*-(3-(cyclohex-1-en-1-yl)-1-phenylprop-2-yn-1-yl) oxime (1h). Yellow solid. Mp: 118.0 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.58-1.66 (m, 4H), 2.10-2.18 (m, 4H), 6.10 (s, 1H), 6.22 (s, 1H), 7.35-7.43 (m, 3H), 7.60 (d, *J* = 6.9 Hz, 2H), 7.75 (d, *J* = 8.7 Hz, 2H), 8.17 (s, 1H), 8.22 (d, *J* = 8.2 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.3, 22.15, 25.60, 28.97, 77.10, 83.34, 90.22, 119.91, 123.90, 127.76, 128.04, 128.50, 128.81, 136.29, 137.55, 138.18, 147.29, 148,33. IR (neat) 3063, 3032, 2930, 2858, 2839, 2219, 1587, 1518, 1494, 1455, 1341, 1296, 1012, 951, 870, 851, 836 cm^{-1}. HRMS (ESI) calcd. For $(M+Na)^+$ 383.1366, found. 383.1366.



(*E*)-4-nitrobenzaldehyde *O*-(3-cyclohexyl-1-phenylprop-2-yn-1-yl) oxime (1i). Yellow solid. Mp: 96.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.17-1.31 (m, 3H), 1.50-1.51 (m, 3H), 1.70-172 (m, 2H), 1.82-1.85 (m, 2H), 2.52 (br, 1H), 6.00 (s, 1H), 7.34-7.42 (m, 3H), 7.60 (d, *J* = 7.3 Hz, 2H), 7.74 (d, *J* = 8.7 Hz, 2H), 8.15 (s, 1H), 8.21 (d, *J* = 8.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 24.69, 25.81, 32.41, 76.86, 77.15, 93.57, 123.90, 127.71, 128.08, 128.44, 128.74, 137.82, 138.27, 147.12, 148.32. IR (neat) 3064, 3033, 2928, 2853, 2231, 1598, 1587, 1519, 1494, 1450, 1341, 1296, 1274, 1108, 951, 852, 836 cm^{-1}. HRMS (ESI) calcd. for $(M+Na)^+$ 385.1523, found 385.1523.

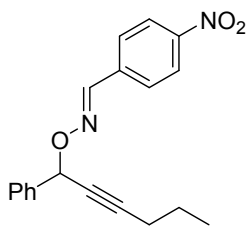


***N*-Benzyl-*N*-methoxy-2-methylbenzenamine (1j).** Yellow solid. Mp: 72.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.22 (d, *J* = 6.9 Hz, 6H), 2.69 (sep, *J* = 6.9 Hz, 1H), 5.98 (s, 1H), 7.34-7.41 (m, 4H), 7.59 (d, *J* = 7.2 Hz, 2H), 7.73 (d, *J* = 8.9 Hz, 2H), 8.15 (s, 1H), 8.21 (d, *J* = 8.9 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.70, 22.79, 76.30, 76.84, 94.93, 123.93, 127.75, 128.06, 128.47, 128.76, 137.84, 138.25, 147.17, 148.35. IR (neat) 3064, 3033, 2971, 2933, 2871, 2254, 1598, 1587, 1519, 1455, 1341, 1319, 1294, 952, 852, 837. HRMS (ESI) calcd. for $(M+Na)^+$ 345.1210, found 345.1210.

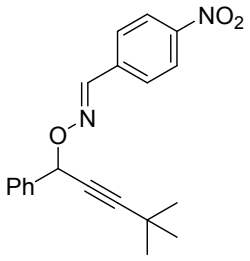


(*E*)-4-nitrobenzaldehyde *O*-(4-methyl-1-phenylpent-2-yn-1-yl) oxime (1k). Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.83 (t, *J* = 7.3 Hz, 3H), 1.21-1.48(m, 4H), 1.74-1.82 (m, 2H), 3.75 (t, *J* = 7.3 Hz, 1H), 6.06 (s, 1H), 7.19-7.29 (m, 3H), 7.36-7.43 (m, 5H), 7.62 (d,

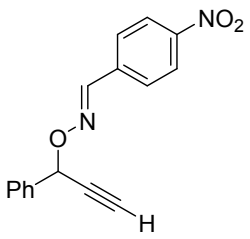
J = 7.3 Hz, 2H), 7.75 (d, *J* = 8.7 Hz, 2H), 8.17(s, 1H), 8.22 (d, *J* = 8.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 22.32, 29.45, 37.93, 38.19, 80.12, 90.87, 123.93, 126.64, 127.41, 127.74, 127.74, 128.17, 128.37, 128.51, 128.87, 137.46, 138.25, 141.73, 147.6, 148.383. IR (neat) 3063, 3030, 2955, 2931, 2859, 2232, 1599, 1588, 1520, 1494, 1454, 1343, 1107, 952, 852, 836 cm^{-1}. HRMS (ESI) calcd. for $(M+Na)^+$ 449.1836, found 449.1836.



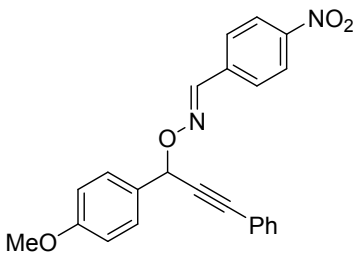
(*E*)-4-nitrobenzaldehyde *O*-(1-phenylhex-2-yn-1-yl) oxime (1l). Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.90 (t, *J* = 7.3 Hz, 3H), 1.59 (sext, *J* = 7.3 Hz, 2H), 2.30 (t, *J* = 6.9 Hz, 2H), 5.98 (s, 1H), 7.34-7.42 (m, 3H), 7.60 (d, *J* = 6.9 Hz, 2H), 7.74 (d, *J* = 8.7 Hz, 2H), 8.16 (s, 1H), 8.21 (d, *J* = 8.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ13.46, 20.89, 21.93, 76.85, 77.32, 89.44, 123.91, 127.75, 128.02, 128.48, 128.77, 137.78, 138.22, 147.22, 148.36. IR (neat) 3064, 3033, 2963, 2933, 2872, 2234, 1598, 1587, 1519, 1495, 1455, 1342, 951, 852, 836 cm^{-1}. HRMS (ESI) calcd. for $(M+Na)^+$ 345.1210, found 345.1209.



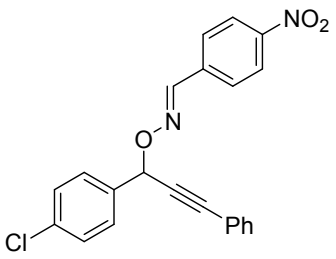
(*E*)-4-nitrobenzaldehyde *O*-(4,4-dimethyl-1-phenylpent-2-yn-1-yl) oxime (1m). Yellow solid. Mp: 102.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.28 (s, 9H), 5.98 (s, 1H), 7.34-7.43 (m, 3H), 7.59 (d, *J* = 6.9 Hz, 2H), 7.74 (d, *J* = 8.7 Hz, 2H), 8.15 (s,1H), 8.22 (d, *J* = 9.2 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 27.60, 30.81, 75.52, 76.81, 97.67, 123.93, 127.70, 128.11, 128.44, 128.74, 137.86, 138.30, 147.04, 148.29. IR (neat) 3064, 3032, 2970, 2930, 2902, 2868, 2241, 1587, 1520, 1455, 1342, 1215, 953, 852, 836 cm^{-1}. HRMS (ESI) calcd. for $(M+Na)^+$ 359.1366, found 359.1366.



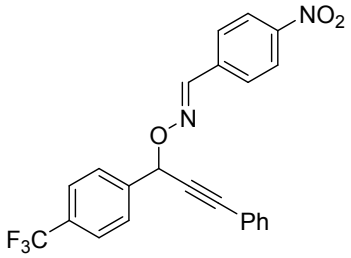
(*E*)-4-nitrobenzaldehyde *O*-(1-phenylprop-2-yn-1-yl) oxime (1n). Yellow solid. Mp: 91.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.77 (d, *J* = 2.3 Hz, 1H), 5.99 (d, *J* = 2.3 Hz, 1H), 7.36-7.44 (m, 3H), 7.61 (d, *J* = 8.7 Hz, 2H), 7.73 (d, *J* = 9.2 Hz, 2H), 8.17 (s, 1H), 8.20 (d, *J* = 8.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 76.03, 80.84, 123.87, 127.82, 127.97, 128.59, 129.11, 136.34, 137.80. IR (neat) 3064, 3033, 2969, 2930, 2901, 2868, 2241, 1587, 1519, 1455, 1341, 952, 852, 836 cm^{-1}. HRMS (ESI) calcd. for $(M+Na)^+$ 303.0740, found 303.0740.



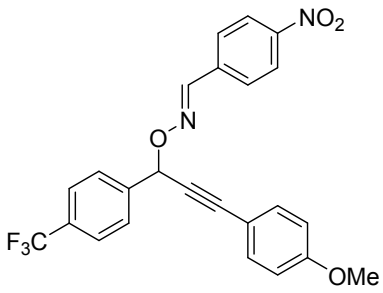
(*E*)-4-nitrobenzaldehyde *O*-(1-(4-methoxyphenyl)-3-phenylprop-2-yn-1-yl) oxime (1o). Yellow solid. Mp: 87.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.83 (s, 3H), 6.13 (s, 1H), 6.95 (d, *J* = 8.7 Hz, 2H), 7.30-7.34 (m, 3H), 7.49-7.52 (m, 2H), 7.61 (d, *J* = 8.7 Hz, 2H), 7.76 (d, *J* = 8.7 Hz, 2H), 8.18 (s, 1H), 8.22 (d, *J* = 9.2 Hz, 2H) ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.30, 76.59, 86.37, 88.01, 122.27, 123.2, 127.78, 128.26, 128.69, 129.30, 129.65, 131.82, 138.16, 147.35, 148.34, 160.13. IR (neat) 3078, 3007, 2960, 2933, 2838, 2228, 1609, 1586, 1513, 1490, 1341, 1305, 1250, 1109, 1031, 942, 839 cm^{-1}. HRMS (ESI) calcd. for $(M+Na)^+$ 409.1159, found 409.1159.



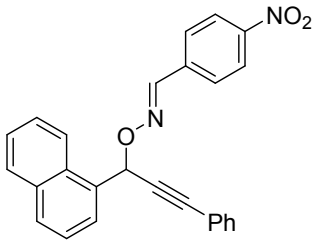
(*E*)-4-nitrobenzaldehyde *O*-(1-(4-chlorophenyl)-3-phenylprop-2-yn-1-yl) oxime (1p). Colorless solid. Mp: 95.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.17 (s, 1H), 7.29-7.35 (m, 3H), 7.40 (d, *J* = 8.2 Hz, 2H), 7.48-7.51 (m, 2H), 7.60 (d, *J* = 8.2 Hz, 2H), 7.75 (d, *J* = 9.2 Hz, 2H), 8.19-8.23 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ76.13, 85.65, 88.58, 122.02, 123.96, 127.86, 128.33, 128.90, 129.47, 131.86, 134.91, 135.89, 137.1, 147.76, 148.53. IR (neat) 3064, 3028, 2899, 2854, 2229, 1597, 1519, 1489, 1296, 1090, 1032, 1015,939, 849, 839, 809 cm^{-1}. HRMS (ESI) calcd. for $(M+Na)^+$ 413.0663, found 413.0663.



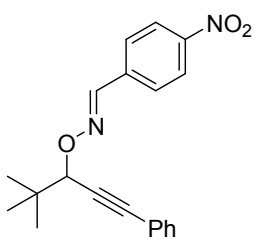
(*E*)-4-nitrobenzaldehyde *O*-(3-phenyl-1-(4-(trifluoromethyl)phenyl)prop-2-yn-1-yl) oxime (1q). Colorless solid. Mp: 79.9 °C ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.25 (s, 1H), 7.31-7.38 (m, 3H), 7.50-7.52 (m, 2H), 7.70 (d, *J* = 8.2 Hz, 2H), 7.78 (t, *J*= 8.2 Hz, 4H), 8.23-8.25 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 76.08, 85.27, 88.89, 121.86, 123.93 (q, *J* = 272.2 Hz), 123.99, 125.61 (q. *J* = 3.8 Hz), 127.92, 128.36, 128.35, 129.01, 131.01 (q, *J* = 32.6 Hz), 131.88, 137.76, 141.26, 148.00, 148.57. IR (neat) 3080, 2939, 2853, 2230, 1598, 1520, 1491, 1418, 1322, 1165, 1124, 1066, 1018, 943, 850 cm^{-1}. HRMS (ESI) calcd. for $(M+Na)^+$ 447.0927, found 447.0927.



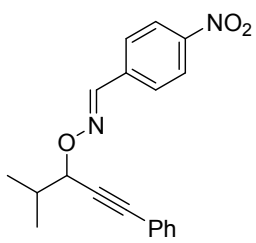
(*E*)-4-nitrobenzaldehyde *O*-(3-(4-methoxyphenyl)-1-(4-(trifluoromethyl)phenyl)prop-2-yn-1-yl) oxime (1r). Colorless solid. Mp: 129.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.83 (s, 3H), 6.17 (s, 1H), 6.96 (d, *J* = 8.7 Hz, 2H), 7.56-7.60 (m, 6H), 7.76 (d, *J* = 8.7 Hz, 2H), 8.19 (s, 1H), 8.22 (d, *J* = 8.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.23, 76.40, 86.50, 88.99, 114.03, 123.79 (q. *J* = 272.2 Hz), 123.94, 125.21 (q. *J* = 3.8 Hz), 126.13, 127.81, 128.89, 129.61, 130.38 (q. *J* = 32.6 Hz), 132.07, 138.01, 147.57, 148.45, 160.29. IR (neat) 3078, 3005, 2936, 2908, 2840, 2908, 2840, 2231, 1613, 1514, 1342, 1321, 1252, 1172, 1125, 1106, 1067, 1017, 944, 841 cm^{-1}. HRMS (ESI) calcd. For $(M+Na)^+$ 477.1033, found.477.1033.



(*E*)-4-nitrobenzaldehyde *O*-(1-(naphthalen-1-yl)-3-phenylprop-2-yn-1-yl) oxime (1s). Yellow solid. Mp: 109.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.86 (s, 1H), 7.28-7.33 (m, 3H), 7.49-7.55 (m, 5H), 7.74-7.77 (m, 2H), 7.89-7.91 (m, 2H), 7.99 (d, *J* = 7.3 Hz, 1H), 8.19-8.21 (m, 3H), 8.34 (d, *J* = 8.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ7.32, 86.27, 88.80, 122.31, 123.91, 123.99, 125.19, 125.94, 126.56, 126.91, 127.87, 128.76, 128.79, 130.03, 130. 95, 131.87, 132.36, 133.99, 138.03, 147.68, 148.41. IR (neat) 3055, 2924, 2851, 2228, 1589, 1519, 1490, 1342, 996, 943 cm^{-1}. HRMS (ESI) calcd. for $(M+Na)^+$ 429.1210, found 429.1210.

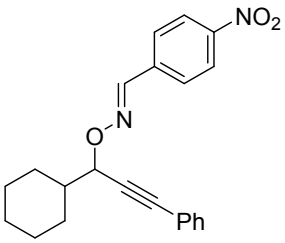


(*E*)-4-nitrobenzaldehyde *O*-(4,4-dimethyl-1-phenylpent-1-yn-3-yl) oxime (1t). Colorless solid. Mp: 71.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.15 (s, 9H), 4.86 (s, 1H), 7.29-7.31 (m, 3H), 7.43-7.47 (m, 2H), 7.78 (d, *J* = 8.7 Hz, 2H), 8.21-8.24 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.00, 35.81, 84.07, 86.75, 86.84, 122.72, 123.96, 127.96, 128.21, 128.37, 131.80, 138.39, 146.60, 148.31. IR (neat) 3081, 2967, 2906, 2870, 2222, 1587, 1520, 1490, 1342, 997, 956, 837 cm^{-1}. HRMS (ESI) calcd. for $(M+Na)^+$ 359.1366, found 359.1366.

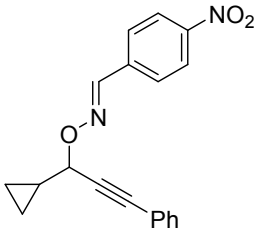


(*E*)-4-nitrobenzaldehyde *O*-(4-methyl-1-phenylpent-1-yn-3-yl) oxime (1u). Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.14 (t, *J* = 6.4

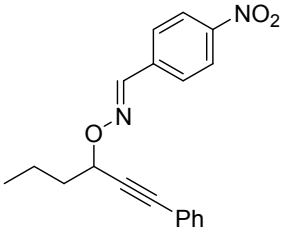
Hz, 6H), 2.27 (sep, *J* = 6.4 Hz, 1H), 4.99 (d, *J* = 6.0 Hz, 1H), 7.28-7.33 (m, 3H), 7.45-7.49 (m, 2H), 7.78 (d, *J* = 8.7 Hz, 2H), 8.20-8.24 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 17.45, 19.58, 32.30, 80.49, 86.02, 86.96, 122.56, 123.93, 127.69, 128.22, 128.44, 131.82, 138.32, 146.84, 148.31. IR (neat) 3081, 2964, 2930, 2907, 2873, 2226, 1588, 1519, 1490, 1341, 987, 957, 838 cm^{-1}. HRMS (ESI) calcd. for $(M+Na)^+$ 345.1210, found 345.1210.



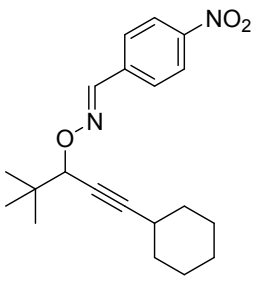
(*E*)-4-nitrobenzaldehyde *O*-(1-cyclohexyl-3-phenylprop-2-yn-1-yl) oxime (1v). Colorless solid. Mp: 94.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.20-1.37 (m, 5H), 1.70-1.97 (m, 6H), 4.98 (d, *J* = 6.0 Hz, 1H), 7.28-7.34 (m, 3H), 7.44-7.49 (m, 2H), 7.79 (d, *J* = 9.2 Hz, 2H), 8.20 (s, 1H), 8.24 (d, *J* = 8.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.75, 25.85, 26.28, 28.09, 28.93, 41.84, 79.83, 86.54, 86.96, 122.57, 123.87, 127.64, 128.16, 128.36, 131.76, 138.30, 146.72, 148.24. IR (neat) 3080, 2926, 2852, 2226, 1587, 1519, 1490, 1444, 1340, 1011, 955, 850, 8333 cm^{-1}. HRMS (ESI) calcd. for $(M+Na)^+$ 385.1523, found 385.1523.



(*E*)-4-nitrobenzaldehyde *O*-(1-cyclopropyl-3-phenylprop-2-yn-1-yl) oxime (1w). Colorless solid. Mp: 61.9 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.63-0.71 (m, 4H), 1.45-1.51 (m, 1H), 5.04 (d, *J* = 6.4 Hz, 1H), 7.28-7.33 (m, 3H), 7.44-7.47 (m, 2H), 7.78 (d, *J* = 8.7 Hz, 2H), 8.21-8.24 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ2.13, 3.48, 14.14, 78.58, 85.58, 85.14, 86.40, 122.26, 123.94, 127.71, 128.22, 128.57, 131.84, 138.31, 146.92, 148.30. IR (neat) 3083, 3008, 2896, 2852, 2231, 1587, 1519, 1490, 1341, 1027, 911, 959, 851, 838 cm^{-1}. HRMS (ESI) calcd. for $(M+Na)^+$ 343.1053, found 343.1053.

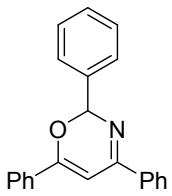


(*E*)-4-nitrobenzaldehyde *O*-(1-phenylhex-1-yn-3-yl) oxime (1x). Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.02 (t, *J* = 7.3 Hz, 3H), 1.62 (sext, *J* = 7.3 Hz, 2H), 1.88-2.05 (m, 2H), 5.17 (t, *J* = 6.9 Hz, 1H), 7.29-7.32 (m, 3H), 7.45-7.47 (m, 2H), 7.79 (d, *J* = 8.7 Hz, 2H), 8.19 (s, 1H), 8.24 (d, *J* = 8.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.81, 18.48, 36.71, 74.97, 86.19, 87.55, 122.52, 123.95, 127.72, 128.22, 128.47, 131.81, 138.33, 146.90, 148.35. IR (neat) 3081, 2960, 2933, 2873, 2232, 1588, 1519, 1490, 1340, 991, 956, 851 cm^{-1}. HRMS (ESI) calcd. for $(M+Na)^+$ 345.1210, found 345.1209.

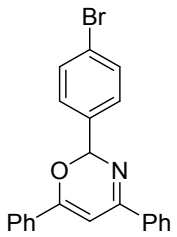


(*E*)-4-nitrobenzaldehyde O-(1-cyclohexyl-4,4-dimethylpent-1-yn-3-yl) oxime (1y). Colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.06 (s, 9H), 1.31-1.49 (m, 6H), 1.69-1.78 (M, 4H), 2.46 (s, 1H), 4.64 (s, 1H), 7.76 (d, J = 8.2 Hz, 2H), 8.17 (s, 1H), 8.23 (d, J = 8.2 Hz) ^{13}C NMR (100 MHz, $CDCl_3$) δ 24.63, 25.88, 25.93, 28.95, 32.49, 32.54, 35.58, 83.98, 91.82, 123.94, 127.58, 138.58, 146.15, 148.17. IR (neat) 2930, 2854, 2230, 1599, 1586, 1521, 1479, 1448, 1393, 1363, 1343, 1194, 1151, 1109, 996, 962, 935, 852, 837 cm^{-1}. HRMS (ESI) calcd. for $(M+Na)^+$ 365.1836, found 365.1836.

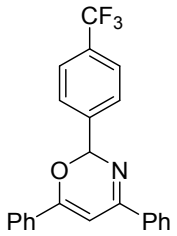
11. Analytical data of 2, 6y, and 7y



2,4,6-triphenyl-2*H*-1,3-oxazine (2a). Reaction time: 72 h. Yield: 26.8 mg (43%). Colorless solid. Decomposed at 100 °C. R_f = 0.23 [hexane/EtOAc = 5:1 (v/v)]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.60 (s, 1H), 6.72 (s, 1H), 7.38-7.48 (m, 9H), 7.78 (d, *J* = 7.3 Hz, 2H), 7.84-7.86 (m, 2H), 7.98-8.00 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ92.989 (br), 95.97, 126.20, 126.85, 127.42, 128.33, 128.47, 128.53, 128.76, 130.52, 131.03, 132.57, 137.07, 139.28, 163.03, 163.42. IR (neat) 3086, 3060, 3033, 2934, 2812, 1629, 1575, 1538, 1492, 1450, 1375, 1338, 1064, 1027, 805, 752 cm^{-1}. HRMS (ESI) calcd. for $(M+H)^+$ 312.1383, found 312.1383.

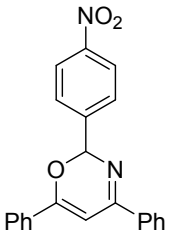


2-(4-bromophenyl)-4,6-diphenyl-2*H*-1,3-oxazine (2b). Reaction time: 48 h. Yield: 59.3 mg (76%). Yellow solid. Decomposed at 90 °C. R_f = 0.49 [hexane/EtOAc = 5:1 (v/v)]. ^{1}H MR (400 MHz, $CDCl_3$) δ 6.49 (s, 1H), 6.71 (s, 1H), 7.40-7.48 (m, 6H), 7.56 (d, *J* = 8.7 Hz, 2H), 7.65 (d, *J* = 8.7 Hz, 2H), 7.79-7.83 (m, 2H), 7.94-7.98 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 91.85 (br), 95.98, 122.82, 126.15, 126.84, 128.53, 128.62, 129.17, 130.69, 131.19, 131.47, 132.27, 136.88, 138.41, 162.61, 163.65. IR (neat) 3085, 3059, 3028, 2827, 1628, 1575, 1541, 1490, 1450, 1373, 1069, 1011, 760, 688 cm^{-1}. HRMS (ESI) calcd. for $(M+H)^+$ 392.0468, found 392.0468.

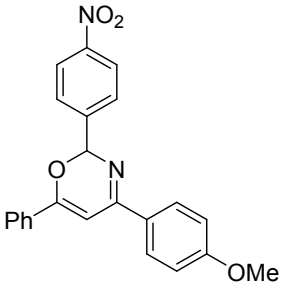


4,6-diphenyl-2-(4-(trifluoromethyl)phenyl)-2*H*-1,3-oxazine (2c). Reaction time: 15 h. Yield: 60.7 mg (80%). Yellow solid. Decomposed at 110 °C. R_f = 0.53 [hexane/EtOAc = 5:1 (v/v)]. ^{1}H MR (400 MHz, $CDCl_3$) δ

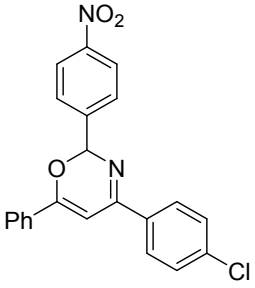
6.53 (s, 1H), 6.73 (s, 1H), 7.41-7.51 (m, 6H), 7.70 (d, *J* = 8.2 Hz, 2H), 7.82-7.85 (m, 2H), 7.90 (d, *J* = 8.2 Hz, 2H), 7.97-7.99 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 90.47 (br), 95.96, 124.12 (q, *J* = 272.2 Hz), 125.32 (q, *J* =3.8 Hz), 126.13, 126.87, 127.71, 128.56, 128.68, 130.36 (q, *J* = 32.6 Hz), 130.79, 131.26, 132.02, 136.77, 143.33, 162.22, 163.79. IR (neat) 3099, 3056, 3036, 2828, 1631, 1576, 1541, 1492, 1451, 1374, 1324, 1165, 1123, 1066, 1019, 759, 688 cm^{-1}. HRMS (ESI) calcd. for $(M+H)^+$ 380.1257, found 380.1257.



2-(4-nitrophenyl)-4,6-diphenyl-2*H*-1,3-oxazine (2d). Reaction time: 8 h. Yield: 66.2 mg (93%). Yellow solid. Decomposed at 118 °C. R_f = 0.50 [hexane/EtOAc = 5:1 (v/v)]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.55 (s, 1H), 6.77 (s, 1H), 7.46-7.52 (m, 6H), 7.84-7.87 (m, 2H), 7.97-8.00 (m, 4H), 8.32 (d, *J* = 8.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 89.61 (br), 96.11, 123.57, 126.10, 126.86, 128.27, 128.60, 128.74, 130.93, 131.40, 131.80, 136.57, 146.38, 148.02, 162.14, 163.991. IR (neat) 3117, 3061, 2928, 2852, 1628, 1575, 1519, 1492, 1450, 1346, 1290, 1097, 1060, 852 cm^{-1}. HRMS (ESI) calcd. for $(M+H)^+$ 357.1234, found 357.1233.

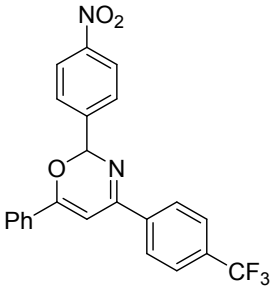


4-(4-methoxyphenyl)-2-(4-nitrophenyl)-6-phenyl-2*H*-1,3-oxazine (2e). Reaction time: 8 h. Yield: 71.0 mg (92%). Yellow solid. Decomposed at 120 °C. R_f = 0.37 [hexane/EtOAc = 5:1 (v/v)]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.86 (s, 3H), 6.48 (s, 1H), 6.74 (s, 1H), 6.98 (d, *J* = 8.7 Hz, 2H), 7.44-7.51 (m, 3H), 7.84 (d, *J* = 6.4 Hz, 2H), 7.96 (d, *J* = 8.2 Hz, 4H), 8.29 (d, *J* = 8.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.4, 89.71 (br), 95.89, 113.83, 123.52, 126.52, 126.04, 128.24, 128.49, 12869, 128.99, 131.27, 131.85, 146.60, 147.89, 161.88, 163.07. IR (neat) 3071, 3005, 2958, 2935, 2838, 1627, 1604, 1574, 1516, 1492, 1347, 1253, 1174, 1031, 852 cm^{-1}. HRMS (ESI) calcd. for $(M+H)^+$ 387.1339, found 387.1339.

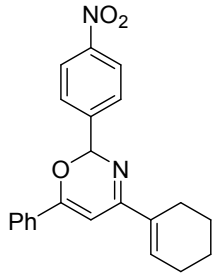


4-(4-chlorophenyl)-2-(4-nitrophenyl)-6-phenyl-2*H*-1,3-oxazine (2f). Reaction time: 8 h. Yield: 73.3 mg (94%). Yellow solid. Decomposed at 120 °C. R_f = 0.50 [hexane/EtOAc = 5:1 (v/v)]. ^{1}H NMR (400 MHz,

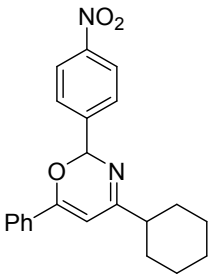
$CDCl_3$) δ 6.52 (s, 1H), 6.72 (s, 1H), 7.45-7.54 (m, 5H), 7.85 (d, *J* = 6.9 Hz, 2H), 7.93-7.98 (m, 4H), 8.32 (d, *J* = 8.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 89.57 (br), 95.64, 123.63, 126.15, 128.24, 128.80, 128.83, 131.59, 134.96, 137.14, 146.18, 148.09, 162.52, 162.96. IR (neat) 2925, 2854, 1626, 1571, 1520, 1491, 1350, 1261, 1092, 1064, 1015, 795, 766 cm^{-1}. HRMS (ESI) calcd. for $(M+H)^+$ 391.0844, found 391.0844.



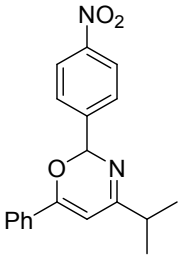
2-(4-nitrophenyl)-6-phenyl-4-(4-(trifluoromethyl)phenyl)-2*H*-1,3-oxazine (2g). Reaction time: 20 h. Yield: 72.9 mg (86%). Yellow solid. Decomposed at 120 °C. R_f = 0.50 [hexane/EtOAc = 5:1 (v/v)]. ^1H NMR (400 MHz, $CDCl_3$) δ 6.55 (s, 1H), 6.75 (s, 1H), 7.46-7.55 (m, 3H),7.74 (d, *J* = 8.2 Hz, 2H), 7.86 (d, *J* = 6.9 Hz, 2H), 7.97 (d, *J* = 8.7 Hz, 2H), 8.10 (d, *J* = 8.2 Hz, 2H), 8.32 (d, *J* = 8.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 89.55 (br), 95.62, 123.62, 123.87 (q. *J* = 272.2 Hz),125.53 (q. *J* = 3.8 Hz), 127.24, 128.21, 128.82, 131.42, 131.72, 132.51 (q. *J* = 32.6 Hz), 139.82, 145.95, 148.09, 162.78, 162.99. IR (neat) 3114, 3056, 2935, 2839, 1632, 1542, 1519, 1492, 1348, 1314, 1162, 1107, 1090, 1066, 852 cm^{-1}. HRMS (ESI) calcd. for $(M+H)^+$ 425.1108, found 425.1107.



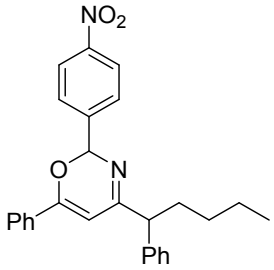
4-(cyclohex-1-en-1-yl)-2-(4-nitrophenyl)-6-phenyl-2*H*-1,3-oxazine (2h). Reaction time: 8 h. Yield: 36.7 mg (51%). Yellow solid. Decomposed at 94 °C. R_f = 0.60 [hexane/EtOAc = 5:1 (v/v)]. ^1H NMR (400 MHz, $CDCl_3$) δ 1.65-1.77 (m, 4H), 2.29 (br, 2H), 2.48 (br, 2H), 6.42 (s, 1H), 6.53 (s, 1H), 6.64 (s, 1H), 7.40-7.48 (m, 3H), 7.76-7.79 (m, 2H), 7.91 (d, *J* = 8.7 Hz), 8.27 (d, *J* = 8.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.88, 22.31, 24.43, 26.12, 90.23 (br), 95.12, 123.48, 125.87, 128.26, 128.60, 130.95, 132.22, 133.19, 136.19, 146.70, 147.85, 164.42. IR (neat) 3059, 2933, 2860, 1624, 1522, 1493, 1346, 1317, 1054, 795 cm^{-1}. HRMS (ESI) calcd. for $(M+H)^+$ 361.1547, found 361.1547.



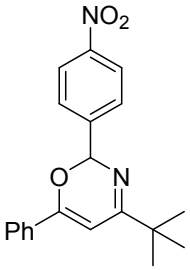
4-cyclohexyl-2-(4-nitrophenyl)-6-phenyl-2*H*-1,3-oxazine (2i). Reaction time: 12 h. Yield: 58.7 mg (81%). Yellow solid. Decomposed at 110 °C. R_f = 0.57 [hexane/EtOAc = 5:1 (v/v)]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.24-1.51 (m, 5H), 1.73-1.76 (m, 1H), 1.84-1.87 (m, 2H), 1.91-1.95 (m, 2H), 2.34-2.42 (m, 1H), 6.19 (s, 1H), 6.29 (s, 1H), 7.40-7.48 (m, 3H), 7.72-7.77 (m, 2H), 7.88 (d, *J* = 8.2 Hz, 2H), 8.27 (d, *J* = 8.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.94, 26.00, 30.43, 46.02, 88.77 (br), 97.07, 128.15, 128.62, 131.06, 131.81, 146.73, 147.91, 160.76, 172.70. IR (neat) 3067, 2927, 2853, 1602, 1555, 1520, 1492, 1449, 1346, 1059, 852 cm^{-1}. HRMS (ESI) calcd. for $(M+H)^+$ 363.1703, found 363.1703.



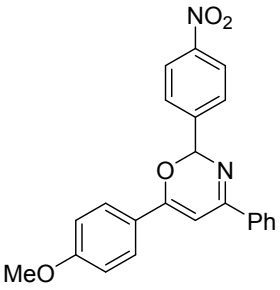
4-isopropyl-2-(4-nitrophenyl)-6-phenyl-2*H*-1,3-oxazine (2j). Reaction time: 15 h. Yield: 34.1 mg (53%). Yellow oil. R_f = 0.47 [hexane/EtOAc = 5:1 (v/v)]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.25 (d, *J* = 6.9 Hz, 6H), 2.70 (sep, *J* = 6.9 Hz, 1H), 6.19 (s, 1H), 6.30 (s, 1H), 7.41-7.47 (m, 3H), 7.76 (d, *J* = 7.3 Hz, 2H), 7.88 (d, *J* = 8.2 Hz, 2H), 8.27 (d, *J* = 8.2 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.10, 35.92, 88.8 (br), 96.5, 123.45, 124.20, 125.80, 128.11, 128.60, 130.38, 131.05, 131.76, 146.66, 147.89, 160.83, 173.33. IR (neat) 3082, 2967, 2931, 2871, 1643, 1556, 1521, 1493, 1450, 1348, 1107, 1059, 853 cm^{-1}. HRMS (ESI) calcd. for $(M+H)^+$ 323.1390, found 323.1390.



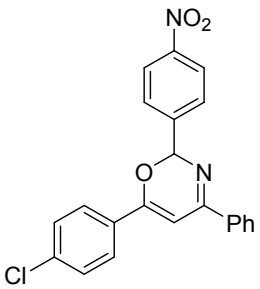
2-(4-nitrophenyl)-6-phenyl-4-(1-phenylpentyl)-2*H*-1,3-oxazine (2k). Reaction time: 8 h. Yield: 52.0 mg (61%). Yellow oil. R_f = 0.57 [hexane/EtOAc = 5:1 (v/v)]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.88 (t, *J* = 7.3 Hz, 3H), 1.27-1.37 (m, 4H), 1.91-1.98 (m, 1H), 2.16 (br, 1H), 6.01 (s, 1H), 6.36 (s, 1H), 7.25-7.44 (m, 8H), 7.65 (d, *J* = 7.8 Hz, 2H), 7.88 (d, *J* = 8.2 Hz, 2H), 8.28 (d, *J* = 8.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 22.81, 29.90, 32.38, 53.17, 88.92 (br), 97.80, 123.68, 125.96, 127.08, 128.32, 128.39, 128.71, 128.79, 131.22, 131.78, 141.11, 146.76, 148.08, 160.77, 170.23. IR (neat) 3061, 3028, 2955, 2931, 2860, 1598, 1557, 1523, 1493, 1451, 1346, 1255, 852 cm^{-1}. HRMS (ESI) calcd. for $(M+H)^+$ 427.2016, found 427.2016.



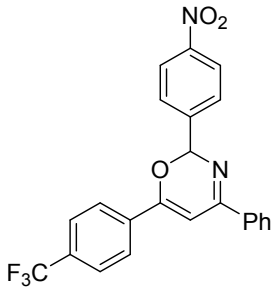
4-(*tert*-butyl)-2-(4-nitrophenyl)-6-phenyl-2*H*-1,3-oxazine (2m). Reaction time: 30 h. Yield: 50.50 mg (75%). colorless oil. R_f = 0.56 [hexane/EtOAc = 5:1 (v/v)]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.28 (s, 9 H), 6.31(s, 1H), 6.34 (s, 1H), 7.41-7.47 (m, 3H), 7.75-7.77 (m, 2H), 7.91 (d, *J* = 8.7 Hz, 2H), 8.28 (d, *J* = 8.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 27.92, 37.78, 88.51, 95.64, 123.46, 125.78, 128.21, 128.64, 130.97, 132.03, 146.84, 147.88, 160.60, 174.88. IR (neat) 3069, 2966, 2867, 1636, 1605, 1552, 1519, 1492, 1477, 1450, 1392, 1364, 1344, 1290, 1261, 1127, 1106, 1061, 1015, 972, 851, 825, 765, 748, 733, 702 cm^{-1}. HRMS (ESI) calcd. for $(M+H)^+$ 337.1552, found 337.1546.



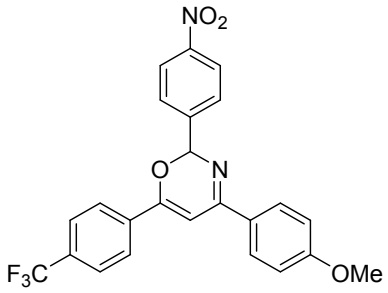
6-(4-methoxyphenyl)-2-(4-nitrophenyl)-4-phenyl-2*H*-1,3-oxazine (2o). Reaction time: 8 h. Yield: 50.2 mg (65%). Yellow solid. Decomposed at 105 °C. R_f = 0.33 [hexane/EtOAc = 5:1 (v/v)]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.87 (s, 3H), 6.49 (s, 1H), 6.67 (s, 1H), 6.97 (d, *J* = 8.7 Hz, 2H), 7.46-7.52 (m,3H), 7.80 (d, *J* = 8.7 Hz, 2H), 7.97 (d, *J* = 8.2 Hz, 2H), 8.30 (d, *J* = 8.2 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.39, 90.0 (br), 94.74, 114.09, 123.49, 124.12, 126.82, 127.96, 128.24, 128.52, 130.76, 136.73, 146.51, 147.94, 162.23, 164.24. IR (neat) 3061, 3006, 2961, 2933, 2839, 1625, 1605, 1519, 1505, 1347, 1255, 1229, 1175, 1060, 1030, 852, 838 cm^{-1}. HRMS (ESI) calcd. for $(M+H)^+$ 387.1339, found 387.1339.



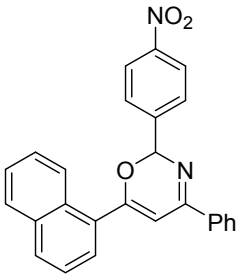
6-(4-chlorophenyl)-2-(4-nitrophenyl)-4-phenyl-2*H*-1,3-oxazine (2p). Reaction time: 8 h. Yield: 71.8 mg (92%). Yellow solid. Decomposed at 130 °C. R_f = 0.63 [hexane/EtOAc = 5:1 (v/v)]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.55 (s, 1H), 6.72 (s, 1H), 7.42-7.53 (m, 5H), 7.77 (d, *J* = 8.7 Hz, 2H), 7.94-7.98 (m, 4H), 8.30 (d, *J* = 8.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 89.96 (br), 96.23, 123.62, 126.84, 127.34, 128.28, 128.65, 129.05, 130.32, 131.04, 136.40, 137.45, 146.15, 148.10, 161.03, 163.78. IR (neat) 3053, 2958, 2925, 2854, 1627, 1538, 1520, 1487, 1348, 1090, 1061, 1013, 824 cm^{-1}. HRMS (ESI) calcd. for $(M+H)^+$ 391.0844, found 391.0844.



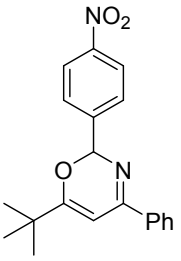
2-(4-nitrophenyl)-4-phenyl-6-(4-(trifluoromethyl)phenyl)-2*H*-1,3-oxazine (2q). Reaction time: 8 h. Yield: 77.2 mg (91%). Yellow solid. Decomposed at 120 °C. R_f = 0.63 [hexane/EtOAc = 5:1 (v/v)]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.61 (s, 1H), 6.82 (s, 1H), 7.48-7.56 (m, 3H), 7.72 (8.2 Hz, 2H), 7.94-8.00 (m, 6H), 8.32 (d, *J* = 8.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 89.75 (br), 97.34, 123.65 (q. *J* = 272.2 Hz), 123.65, 125.72 (q. *J* = 3.8 Hz), 126.25, 126.84, 128.28, 128.70, 131.19, 132.80, 135.29, 136.20, 145.96, 148.14, 160.34, 163.44. IR (neat) 3066, 2935, 2853, 1632, 1544, 1522, 1417, 1348, 1322, 1169, 1126, 1067, 1015, 851. cm^{-1}. HRMS (ESI) calcd. for $(M+H)^+$ 425.1108, found 3425.1107.



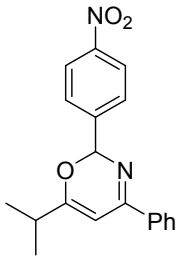
4-(4-methoxyphenyl)-2-(4-nitrophenyl)-6-(4-(trifluoromethyl)phenyl)-2*H*-1,3-oxazine (2r). Reaction time: 8 h. Yield: 84.5 mg (93%). Yellow solid. Decomposed at 120 °C. R_f = 0.37 [hexane/EtOAc = 5:1 (v/v)]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.87 (s, 3H), 6.48 (s, 1H), 6.64 (s, 1H), 6.97 (d, *J* = 8.7 Hz, 2H), 7.72 (d, *J* = 8.2 Hz, 2H), 7.80 (d, *J* = 9.2 Hz, 2H), 7.96 (d, *J* = 8.7 Hz, 2H), 8.08 (d, *J* = 8.2 Hz, 2H), 8.29 (d, *J* = 8.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.43, 89.88 (br), 94.29, 114.21, 123.59, 123.78, 123.90 (q, *J* = 272.2 Hz), 125.47 (q, *J* = 3.8 Hz), 127.23, 128.10, 128.22, 132.38 (q. *J* = 32.6 Hz), 140.07, 146.12, 148.07, 162.53, 162.93, 163.27. IR (neat) 3081, 3006, 2936, 2841, 1625, 1605, 1520, 1505, 1348, 1322, 1258, 1176, 1123, 1093, 1068, 1016, 853 cm^{-1}. HRMS (ESI) calcd. for $(M+H)^+$ 455.1213, found 455.1213.



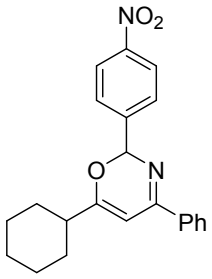
6-(naphthalen-1-yl)-2-(4-nitrophenyl)-4-phenyl-2*H*-1,3-oxazine (2s). Reaction time: 8 h. Yield: 75.5 mg (93%). Yellow solid. Decomposed at 120 °C. R_f = 0.47 [hexane/EtOAc = 5:1 (v/v)]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.64 (s, 1H), 6.72 (s, 1H), 7.47-7.59 (m, 6H), 7.75 (d, *J* = 7.3 Hz, 2H), 7.90-7.92 (m, 1H), 7.96-8.03 (m, 5H), 8.26-8.30 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 90.65 (br), 101.73, 123.59, 125.01, 126.36, 126.89, 127.13, 127.72, 128.36, 128.65, 128.72, 130.62, 131.06, 131.32, 133.76, 136.28, 146.11, 148.04, 163.78, 164.71. IR (neat) 3060, 2949, 2812, 1629, 1578, 1519, 1372, 1345, 1034, 851.4, 801.3 cm^{-1}. HRMS (ESI) calcd. for $(M+H)^+$ 407.1390, found 407.1390.



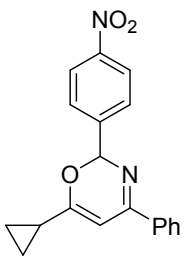
6-(*tert*-butyl)-2-(4-nitrophenyl)-4-phenyl-2*H*-1,3-oxazine (2t). Reaction time: 62 h. Yield: 60.6 mg (90%). Yellow oil. R_f = 0.60 [hexane/EtOAc = 5:1 (v/v)]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.24 (s, 9H), 6.10 (s, 1H), 6.27 (s, 1H), 7.42-7.50 (m, 3H), 7.88-7.92 (m, 4H), 8.29 (d, *J* = 8.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 27.54, 35.85, 89.42 (br), 94.39, 123.46, 126.78, 128.23, 128.50, 130.74, 136.75, 146.59, 147.94, 164.01, 175.62. IR (neat) 3111, 3062, 2968, 2906, 2871, 1630, 1606, 1580, 1520, 1347, 1267, 1108, 1033, 1014, 852 cm^{-1}. HRMS (ESI) calcd. for $(M+H)^+$ 337.1547, found 337.1547.



6-isopropyl-2-(4-nitrophenyl)-4-phenyl-2*H*-1,3-oxazine (2s). Reaction time: 21 h. Yield: 25.8 mg (40%). Yellow oil. R_f = 0.57 [hexane/EtOAc = 5:1 (v/v)]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.21 (t, *J* = 6.9 Hz, 6H), 2.57 (sep, *J* = 6.9 Hz, 1H), 6.05 (s, 1H), 6.33 (s, 1H), 7.39-7.49 (m, 3H), 7.84-7.91 (m, 4H), 8.27 (d, *J* = 8.7 Hz, 2H. ^{13}C NMR (100 MHz, $CDCl_3$) δ 19.71, 32.54, 89.93, 95.42, 123.41, 123.74, 126.72, 128.22, 128..46, 128.83, 130.72 136.56, 146.51, 147.91, 163.60, 173.67. IR (neat) 3112, 3064, 2969, 2932, 2871, 1708, 1605, 1573, 1524, 1487, 1346, 853 cm^{-1}. HRMS (ESI) calcd. for $(M+H)^+$ 323.1390, found 323.1390.

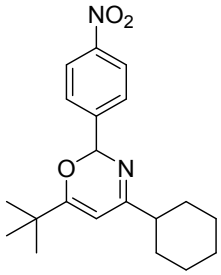


6-cyclohexyl-2-(4-nitrophenyl)-4-phenyl-2*H*-1,3-oxazine (2u). Reaction time: 20 h. Yield: 47.1 mg (65%). Yellow solid. Decomposed at 80 °C. R_f = 0.62 [hexane/EtOAc = 5:1 (v/v)]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.17-1.44 (m, 5H), 1.71-1.74 (m, 1H), 1.81-1.84 (m, 2H), 1.94-1.97 (m, 2H), 2.21-2.28 (m, 1H), 6.03 (s, 1H), 6.29 (s, 1H), 7.41-7.49 (m, 3H), 7.83-7.91 (m, 4H), 8.27 (d, *J* = 8.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.81, 30.12, 42.06, 89.43 (br), 95.75, 123.44, 126.75, 128.26, 128.47, 130.72, 136.63, 146.59, 147.91, 163.69, 172.80. IR (neat) 3110, 3060, 2928, 2853, 1633, 1604, 1520, 1486, 1447, 1345, 1069, 1037, 1014, 1000, 852 cm^{-1}. HRMS (ESI) calcd. for $(M+H)^+$ 363.1703, found 363.1703.

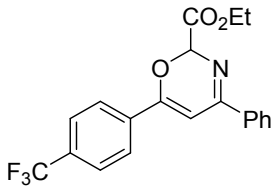


6-cyclopropyl-2-(4-nitrophenyl)-4-phenyl-2*H*-1,3-oxazine (2w). Reaction time: 24 h. Yield: 38.4 mg (60%). Yellow oil. R_f = 0.33 [hexane/EtOAc = 5:1 (v/v)]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.88-0.92 (m, 2H), 1.01-1.04 (m, 2H), 1.71-1.78 (m, 1H), 6.18 (s, 1H), 6.61 (br, 1H), 7.42-7.48 (m, 3H), 7.85-7.88 (m, 4H), 8.27 (d, *J* = 9.2 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 7.93, 15.27, 98.48, 123.53, 126.73, 128.43, 128.49,

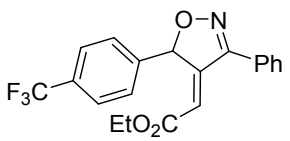
130.62, 136.47, 145.43, 148.19, 162.95. IR (neat) 3114, 3081, 3009, 2855, 1706, 1605, 1566, 1521, 1479, 1445, 1385, 1344, 1319, 1282, 1197, 1107, 1059, 1014, 917, 852 cm^{-1}. HRMS (ESI) calcd. for $(M+H)^+$ 321.1234, found 321.1234.



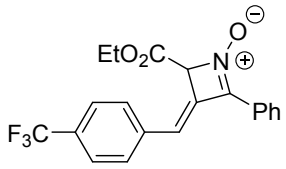
6-(tert-butyl)-4-cyclohexyl-2-(4-nitrophenyl)-2*H*-1,3-oxazine (2y). Reaction time: 72 h. Yield: 49.3 mg (72%). Yellow oil. R_f = 0.60 [hexane/EtOAc = 5:1 (v/v)]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.13 (s, 9H), 1.19-1.41 (m, 5H), 1.68-1.85 (m, 5H), 2.21-2.27 (m, 1H), 5.47 (s, 1H), 5.99 (s, 1H), 7.78 (d, *J* = 8.7 Hz, 2H), 8.23 (d, *J* = 8.7Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.91, 25.97, 27.46, 30.35, 35.44, 45.90, 88.05, 95.27, 123.38, 128.12, 146.86, 147.76, 172.85. IR (neat) 2930, 2854, 1741, 1696, 1643, 1604, 1567, 1524, 1479, 1449, 1346, 1265, 1105, 1014, 916, 852 cm^{-1}. HRMS (ESI) calcd. for $(M+H)^+$ 343.2016, found 343.2016.



ethyl 4-phenyl-6-(4-(trifluoromethyl)phenyl)-2*H*-1,3-oxazine-2-carboxylate (2z). Reaction time: 7 h. Yield: 48.8 mg (65%). Yellow solid. Mp: 65.8 °C. R_f = 0.32 [hexane/EtOAc = 5:1 (v/v)]. ^{1}H MR (400 MHz, $CDCl_3$) δ 1.34 (t, *J* = 7.3 Hz, 3H), 4.35 (q. *J* = 7.3 Hz, 2H), 6.18 (s, 1H), 6.65 (s, 1H), 7.44-7.52 (m, 3H), 7.71 (d, *J* = 8.2 Hz, 2H), 7.91-7.97 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.11, 62.03, 86.77, 96.78, 123.70 (q. *J* = 272.2 Hz), 125.58 (q. *J* = 2.9 Hz), 126.59,126.90, 128.57, 131.09, 132.71 (q. *J* = 32.6 Hz), 135.3, 136.1. IR (neat) 3060, 2984, 2937, 1747, 1636, 1618, 1577, 1550, 1416, 1380, 1322, 1205, 1169, 1114, 1068, 1015, 852 cm^{-1}. HRMS (ESI) calcd. for $(M+H)^+$ 376.1155, found 376.1155.



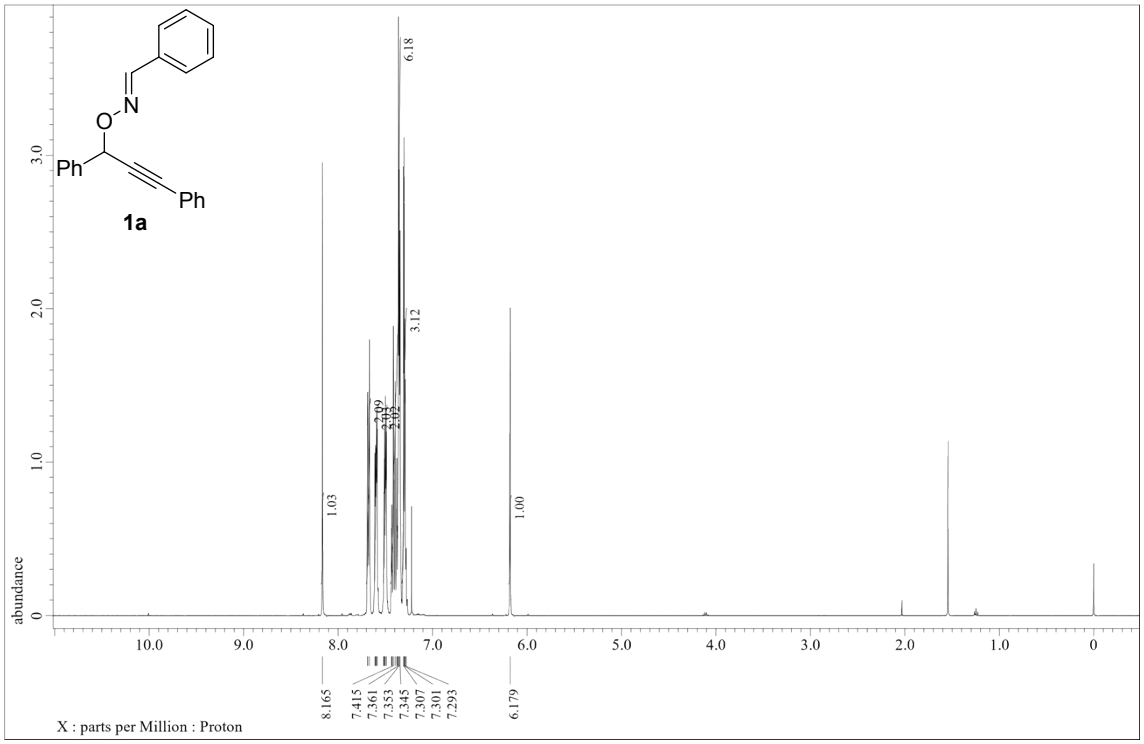
2-(Ethyl (*Z*)-2-(3-phenyl-5-(4-(trifluoromethyl)phenyl)isoxazol-4(5*H*)-ylidene)acetate (6z). Reaction time: 1 h. Yield: 42.0 mg (56%). Colorless solid. Mp: 138.2 °C. R_f = 0.57 [hexane/EtOAc = 5:1 (v/v)]. ^{1}H MR (400 MHz, $CDCl_3$) δ 1.18 (t, *J* = 7.3 Hz, 3H), 4.14-4.05 (m, 2H), 6.36 (d, *J* = 3.2 Hz, 1H), 6.82 (d, *J* = 3.2 Hz, 1H), 7.55-7.48 (m, 5H), 7.66-7.61 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.00, 61.04, 86.90, 116.02, 123.89 (q, *J* = 272.2 Hz), 125.58 (q, *J* = 3.8 Hz), 127.04, 127.95, 128.28, 129.15, 130.56, 130.71 (q, *J* = 32.6 Hz), 141.23, 154.70, 157.43, 165.16. IR (neat) 3062, 2983, 2938, 1710, 1643, 1618, 1445, 1419, 1368, 1323, 1269, 1203, 1166, 1124, 1112, 1067, 1036, 1019, 900, 881, 833 cm^{-1}. HRMS (ESI) calcd. for $(M+Na)^+$ 398.0975, found 398.0975.

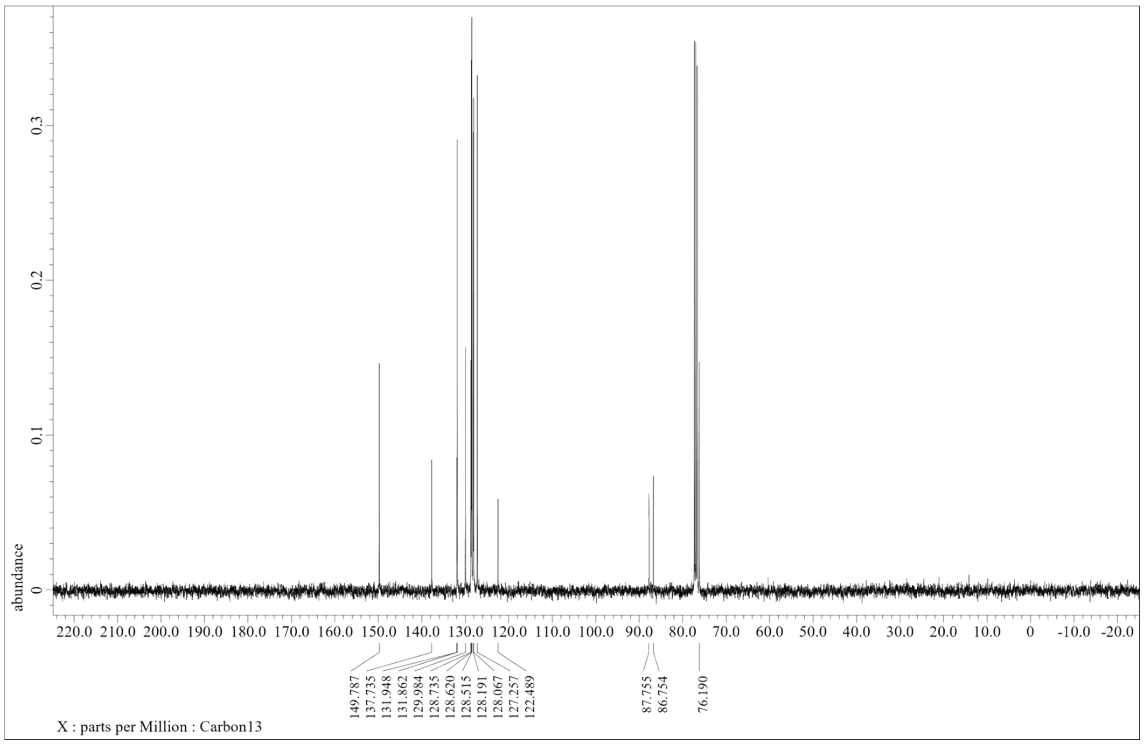


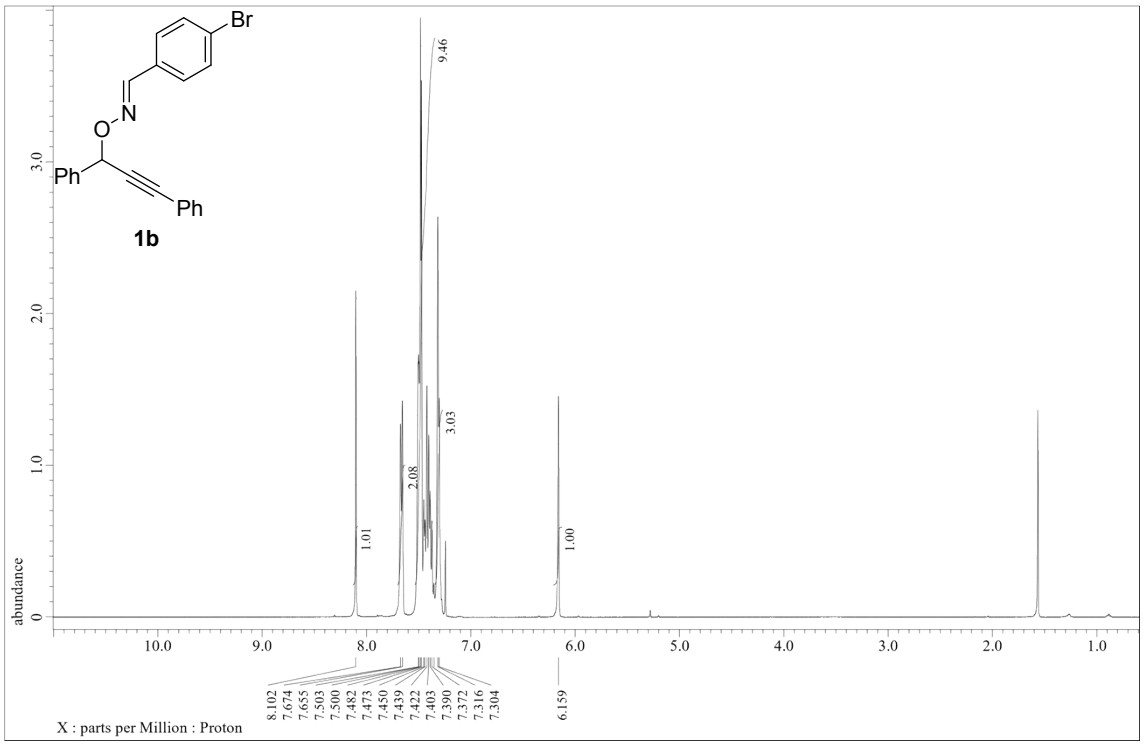
(*E*)-2-(ethoxycarbonyl)-4-phenyl-3-(4-

(trifluoromethyl)benzylidene)-2,3-dihydroazete 1-oxide (7z). Reaction time: 48 h. Yield: 34.7 mg (46%). Colorless solid. Mp: 121.1 °C. R_f = 0.27 [hexane/EtOAc = 5:1 (v/v)]. ^{1}H MR (400 MHz, $CDCl_3$) δ 1.14 (t, *J* = 7.3 Hz, 3H), 4.22 (q, *J* = 7.3 Hz, 2H), 5.83 (s, 1H), 6.90 (s, 1H), 7.45-7.55 (m, 5H), 7.62 (d, *J* = 8.2 Hz, 2H), 8.12-8.14 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.80, 62.72, 81.98, 116.50, 123.91 (q, *J* = 272.2 Hz), 125.69 (q, *J* = 3.8 Hz), 126.38, 127.15, 127.95, 128.91, 129.84 (q, J = 32.6 Hz), 130.95, 137.78, 152.91, 164.39. IR (neat) 3063, 2984, 2940, 2907, 1742, 1688, 1615, 1577, 1549, 1493, 1450, 1414, 1370, 1323, 1261, 1187, 1166, 1121, 1111, 1067, 1042, 1014, 868 cm^{-1}. HRMS (ESI) calcd. for $(M+Na)^+$ 398.0975, found 398.0975.

12. ^{1}H, ^{13}C NMR and NOE charts of 1, 2, 6z and 7z



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O
Ph
Ph
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3.03
2.08
1.01
1.00
abundance
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8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
8.102
7.674
7.655
7.503
7.500
7.482
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7.439
7.422
7.403
7.390
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7.316
7.304
6.159
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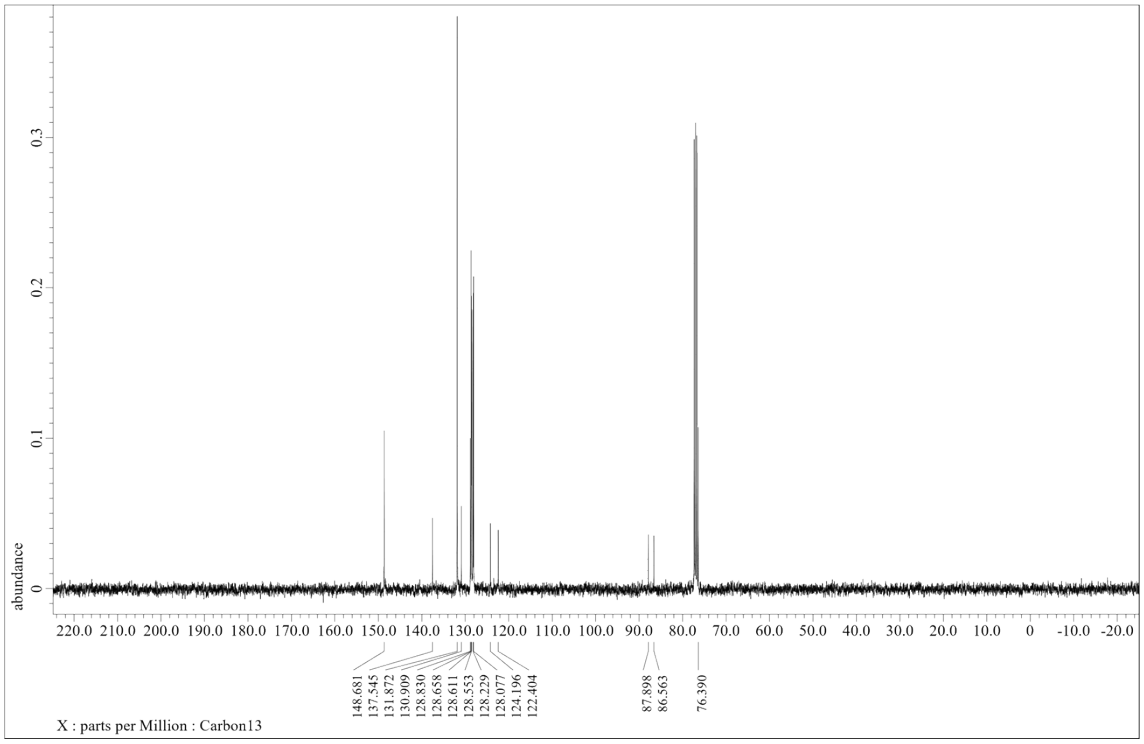
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137.545
131.872
130.909
128.830
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128.553
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128.077
124.196
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87.898
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76.390
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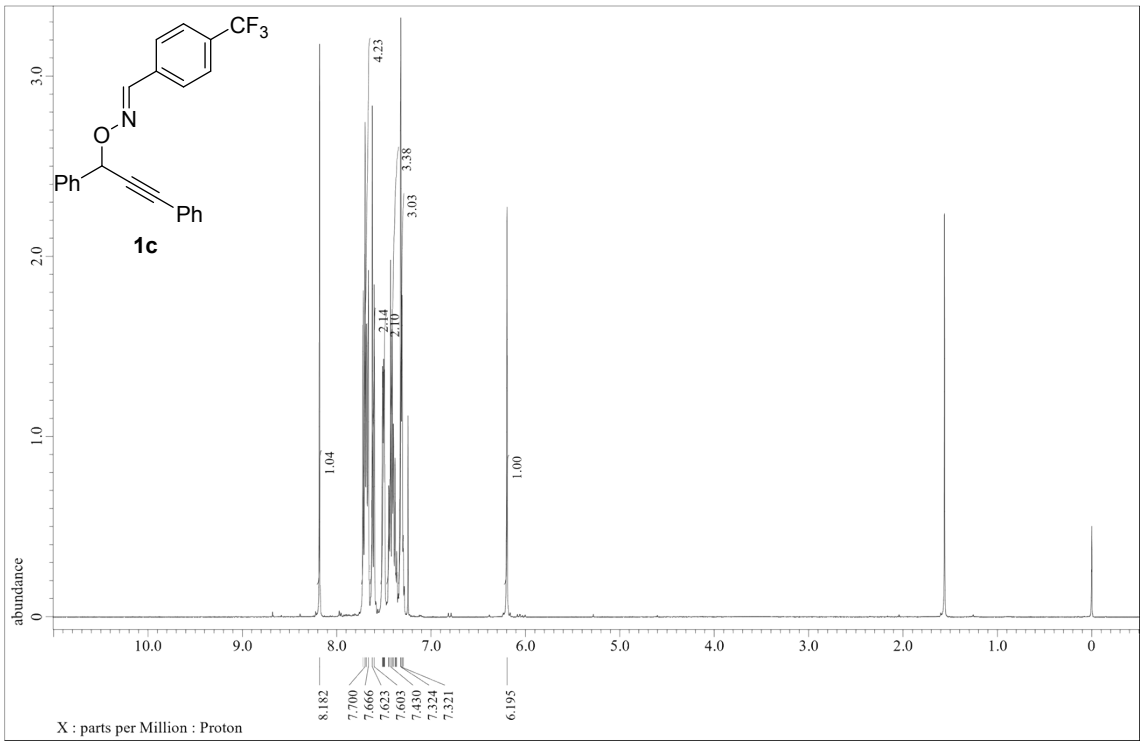
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Ph
Ph
1c
abundance
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1.04
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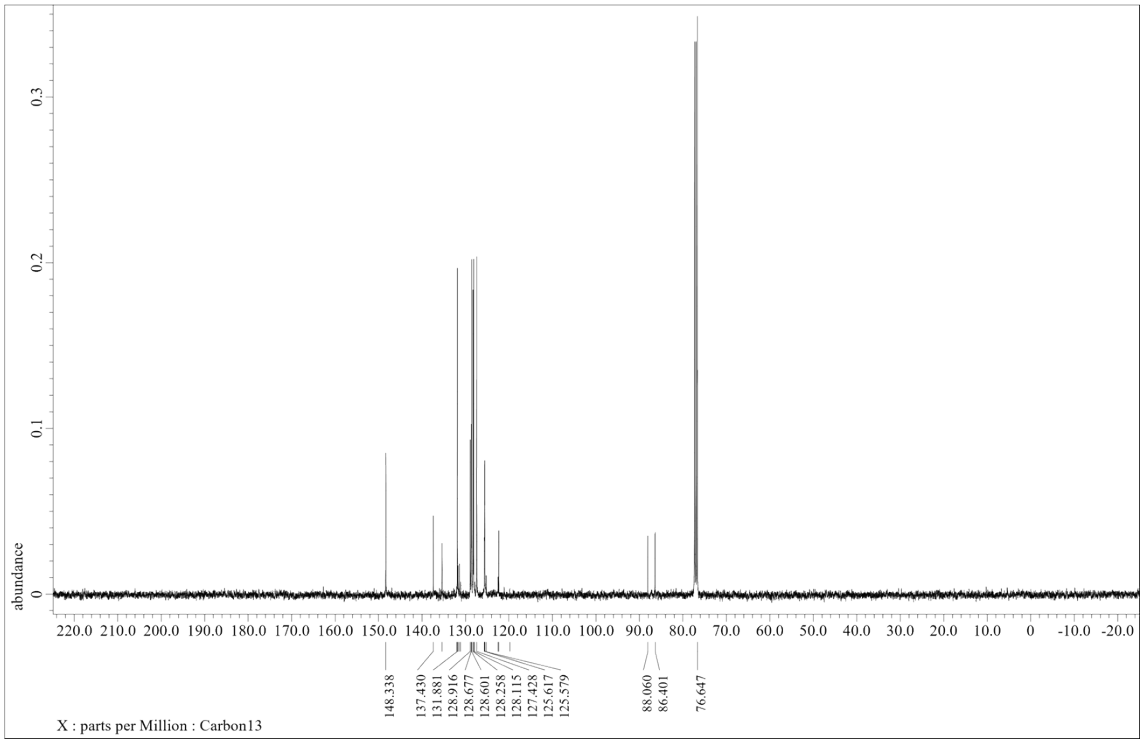
X : parts per Million : Proton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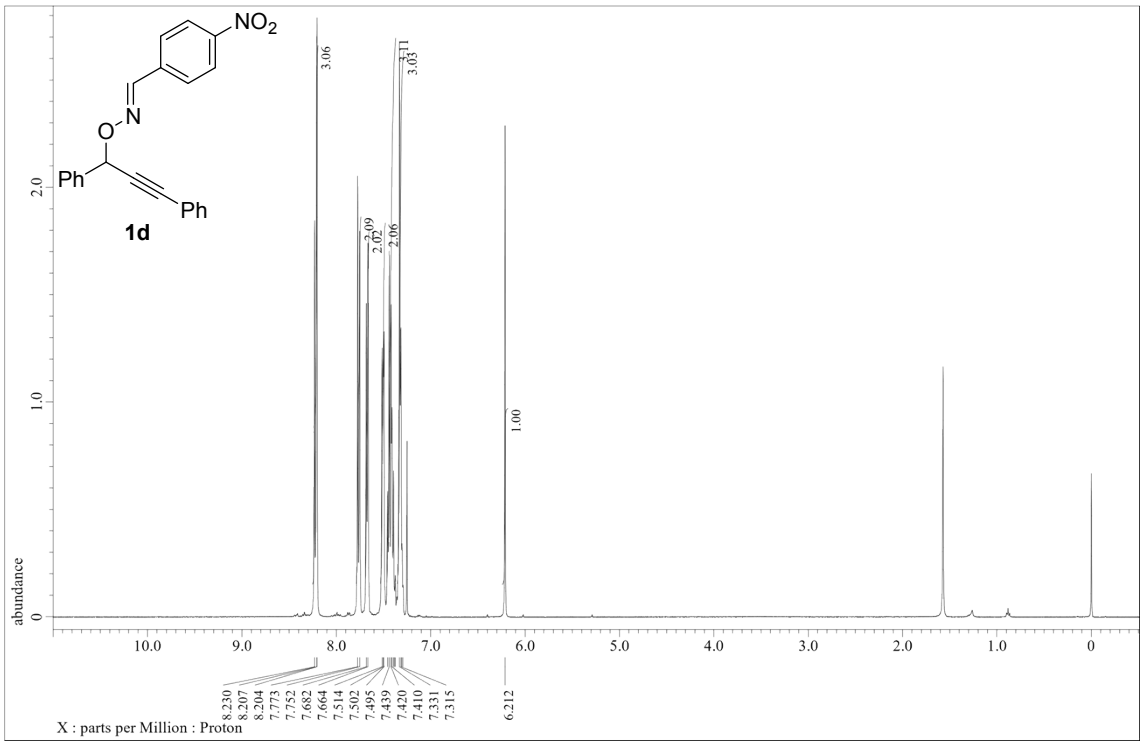
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Ph
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3.11
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2.06
1.00
abundance
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8.207
8.204
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7.752
7.682
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7.502
7.495
7.439
7.420
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7.331
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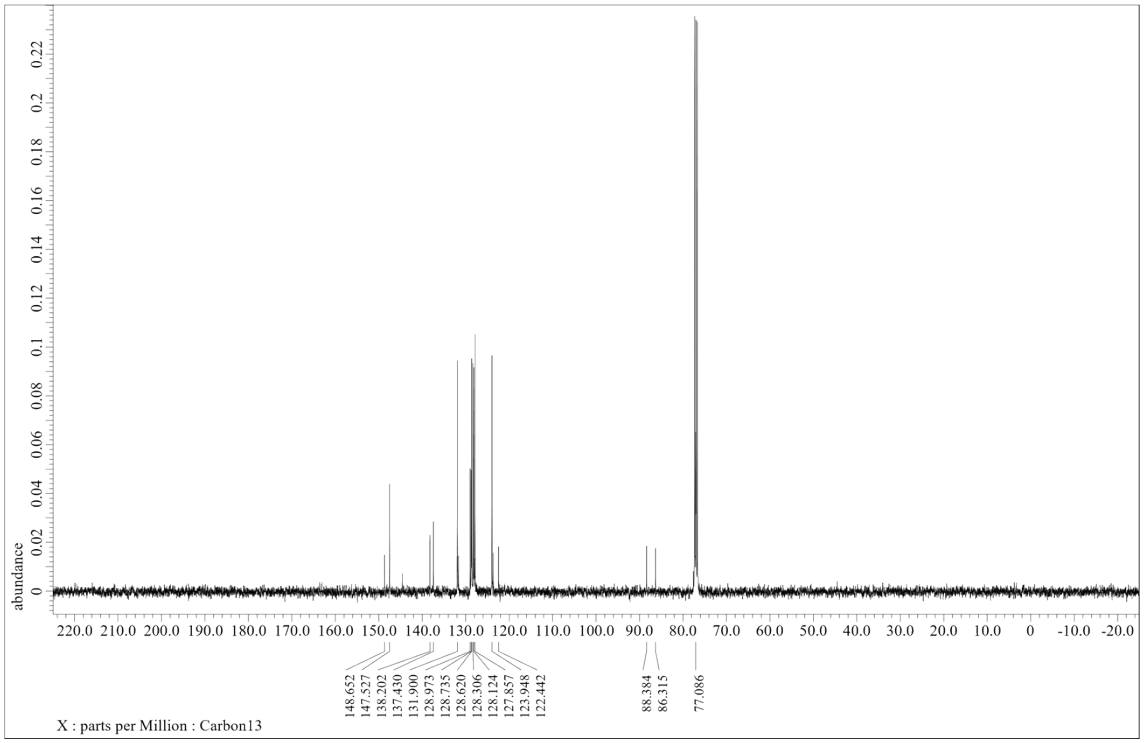
X : parts per Million : Proton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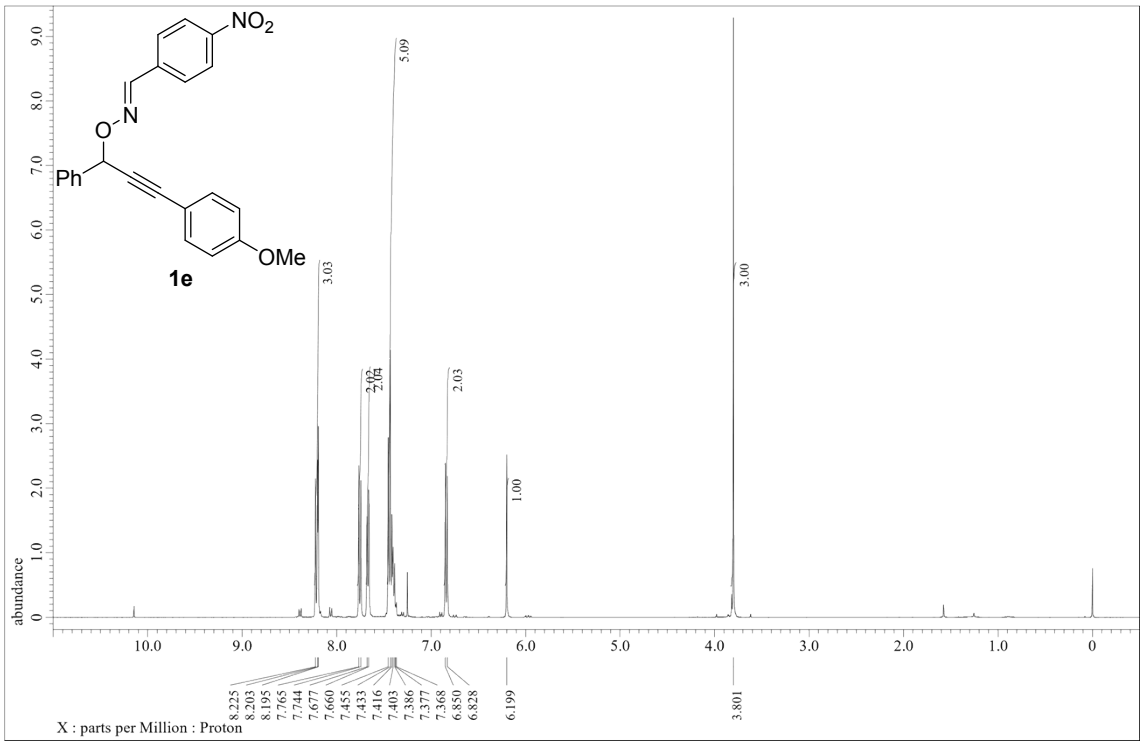
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Ph
OMe
1e
abundance
X : parts per Million : Proton
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7.677
7.660
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3.03
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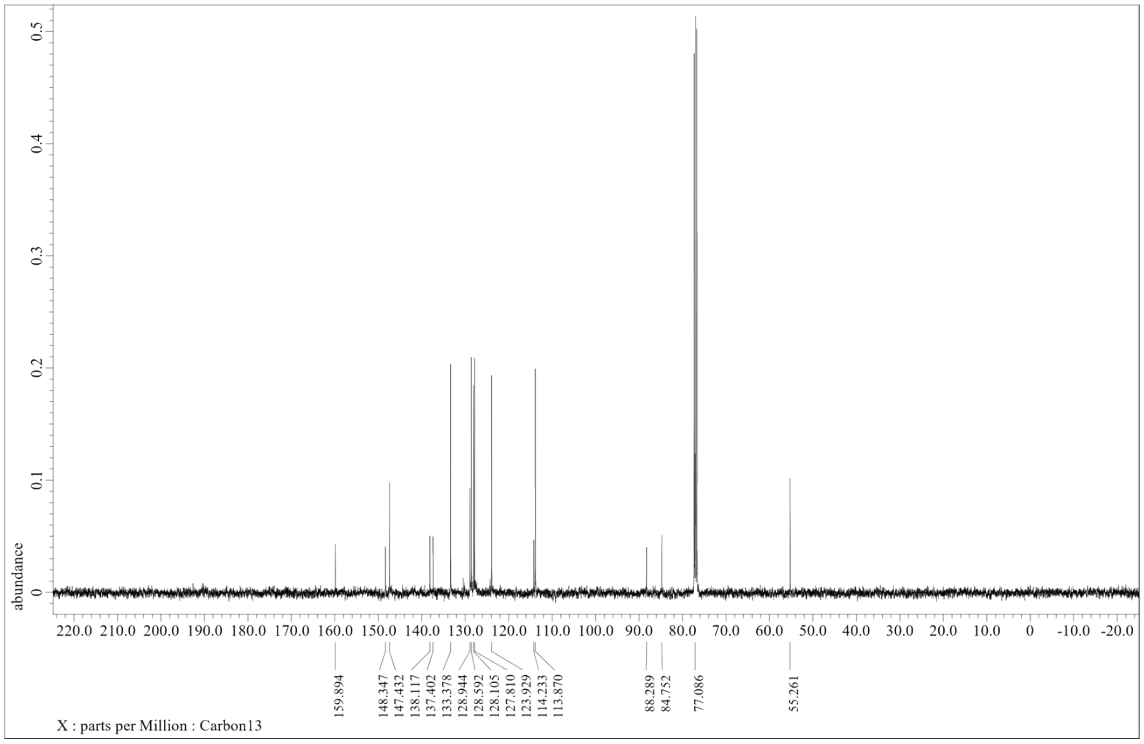
2.03
1.00


abundance
X : parts per Million : Carbon13
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113.870
88.289
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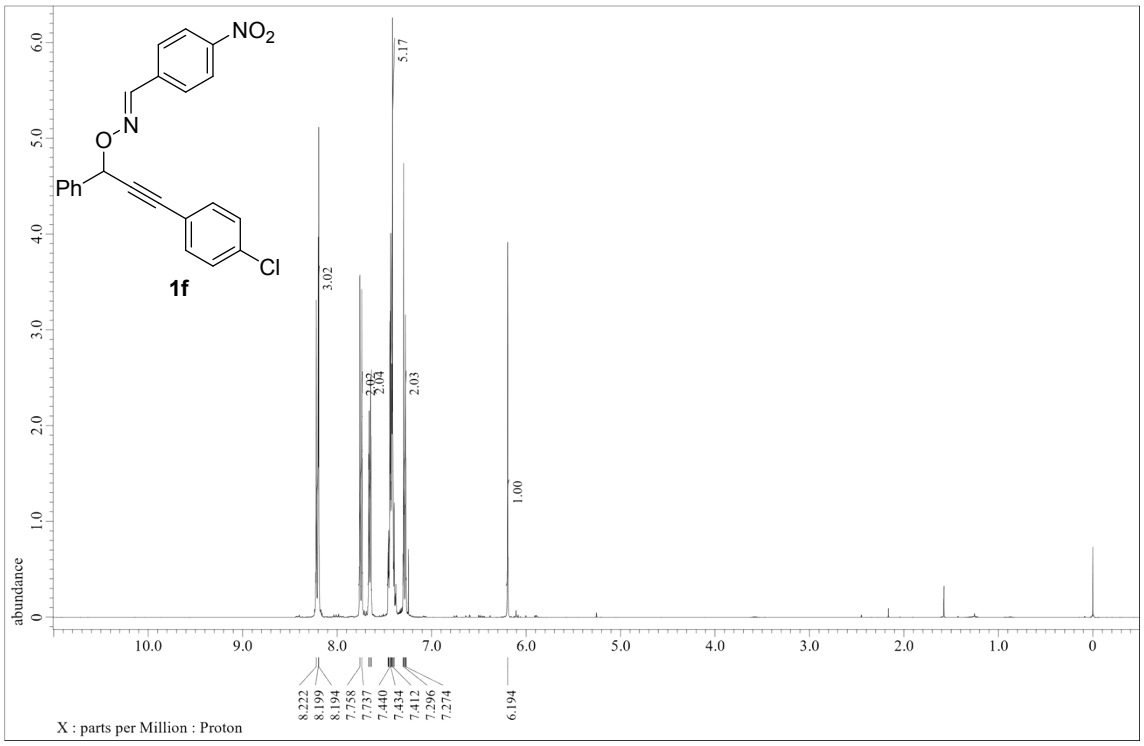
55.261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O
Ph
Cl
1f
abundance
X : parts per Million : Proton
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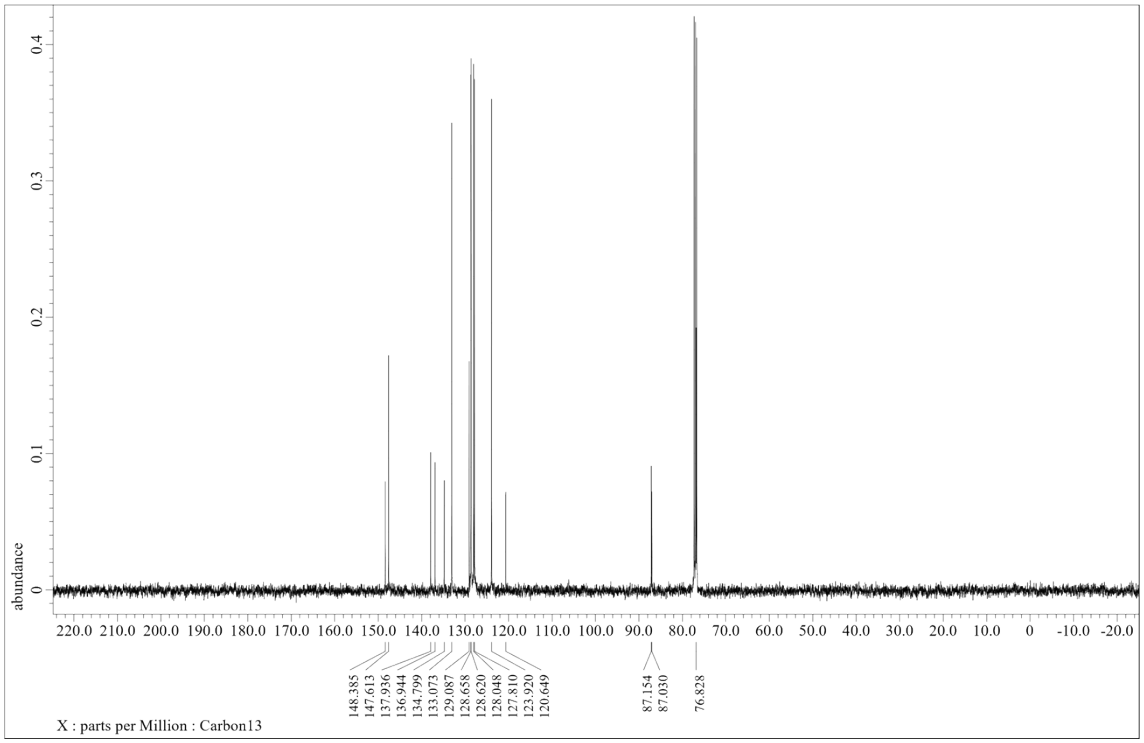
5.17
3.02
2.05
2.04
2.03
1.00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X : parts per Million : Carbon13
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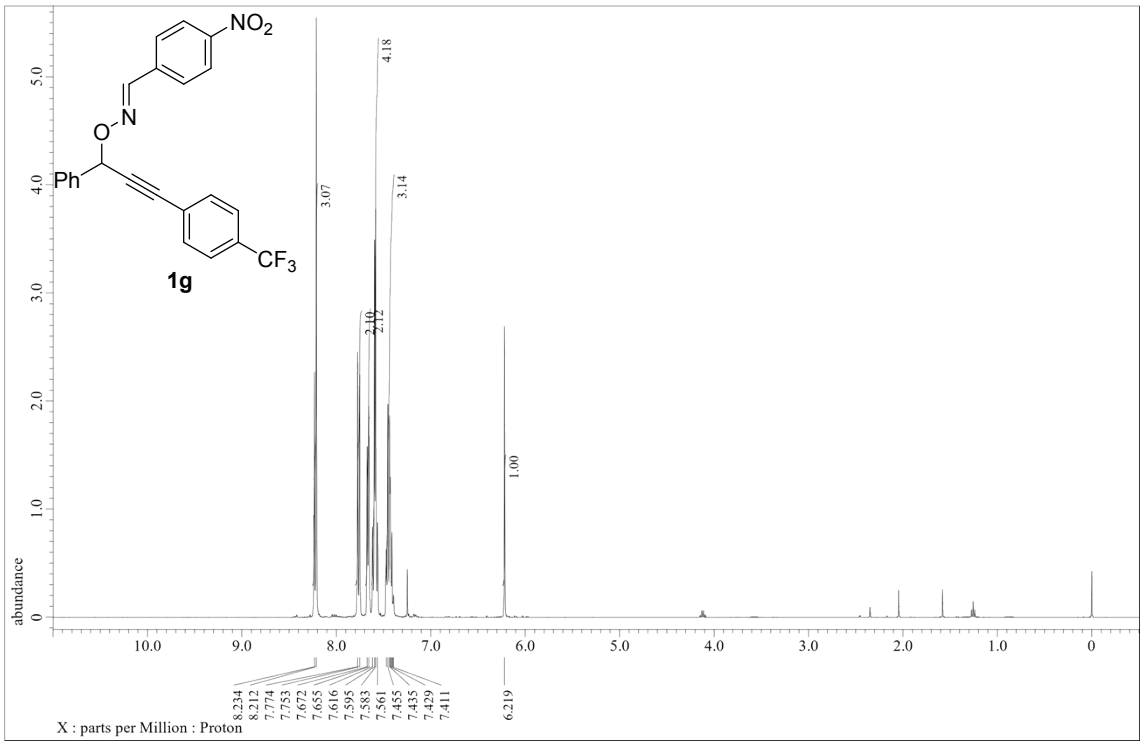
87.154
87.030
76.828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1g
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1.00
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8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
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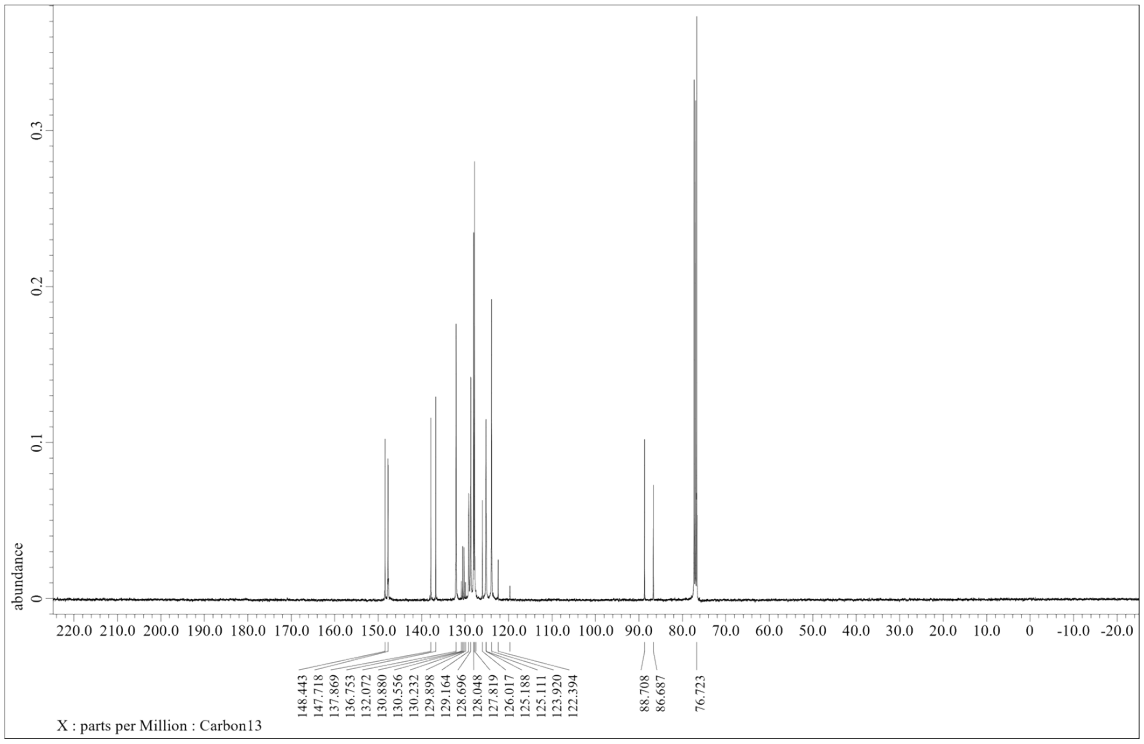
X : parts per Million : Proton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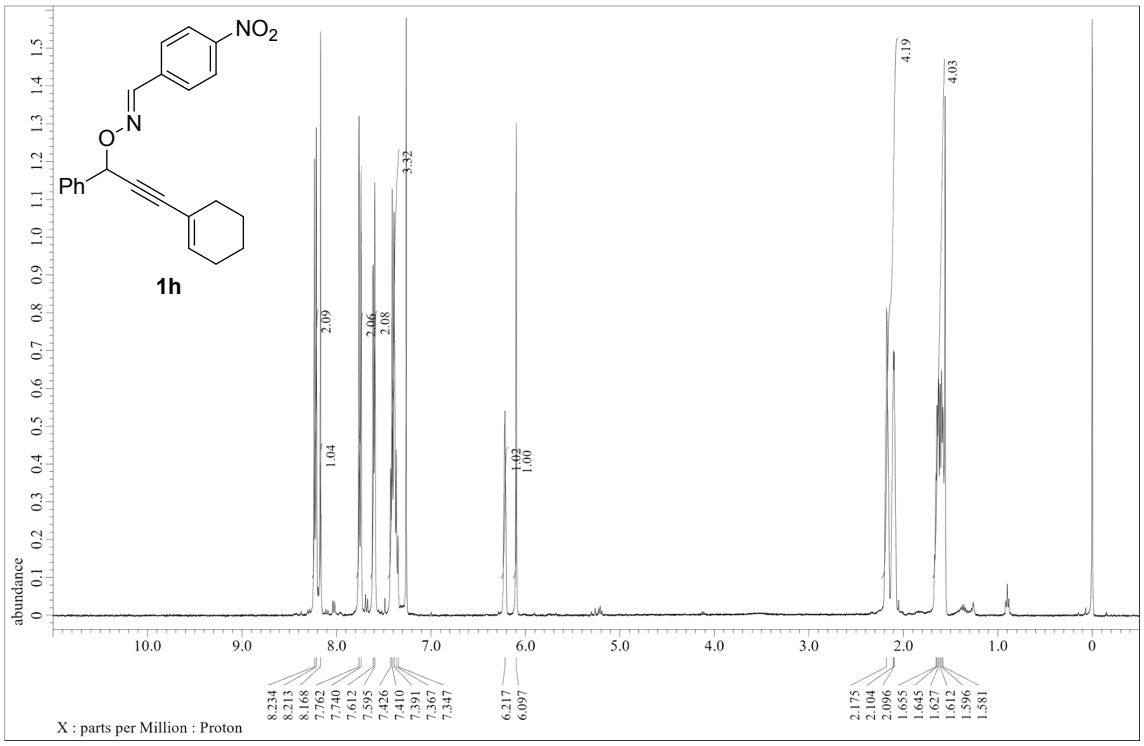
X : parts per Million : Carbon13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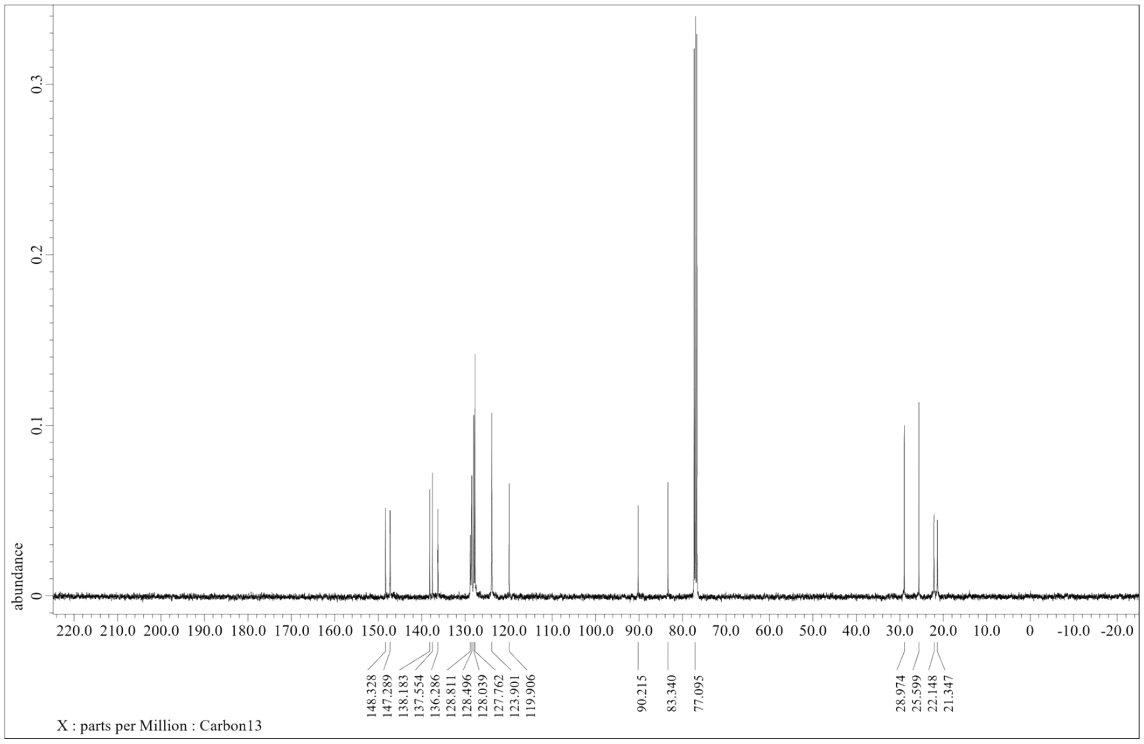
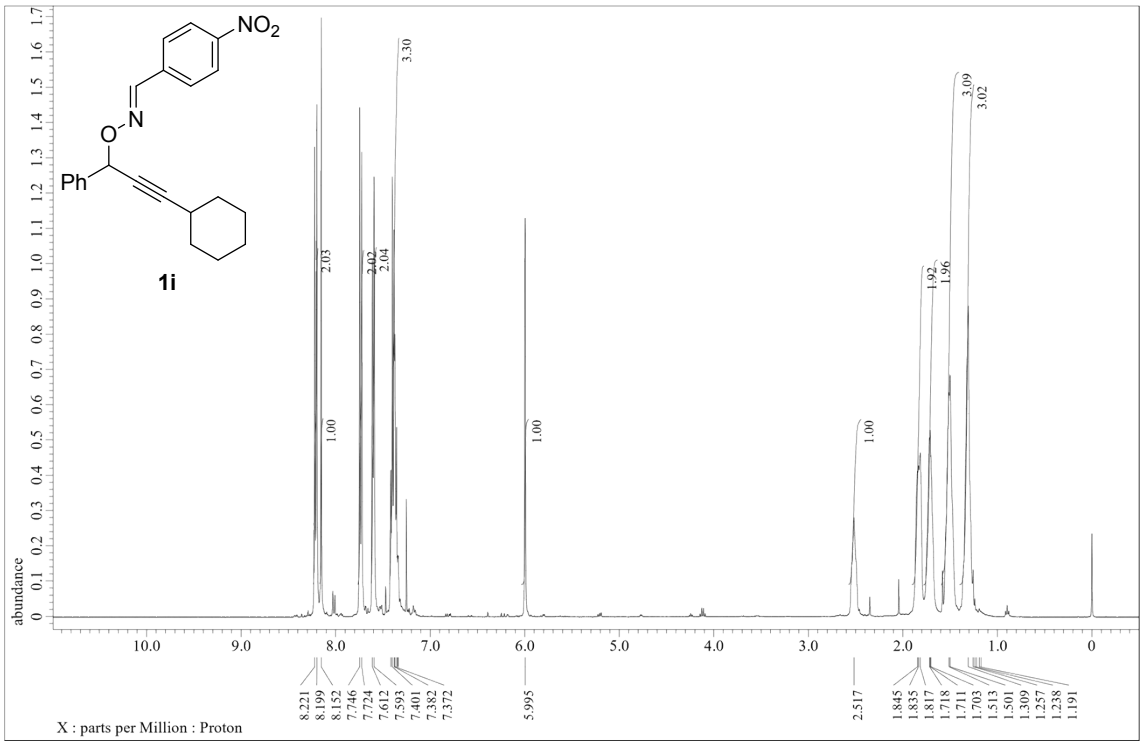
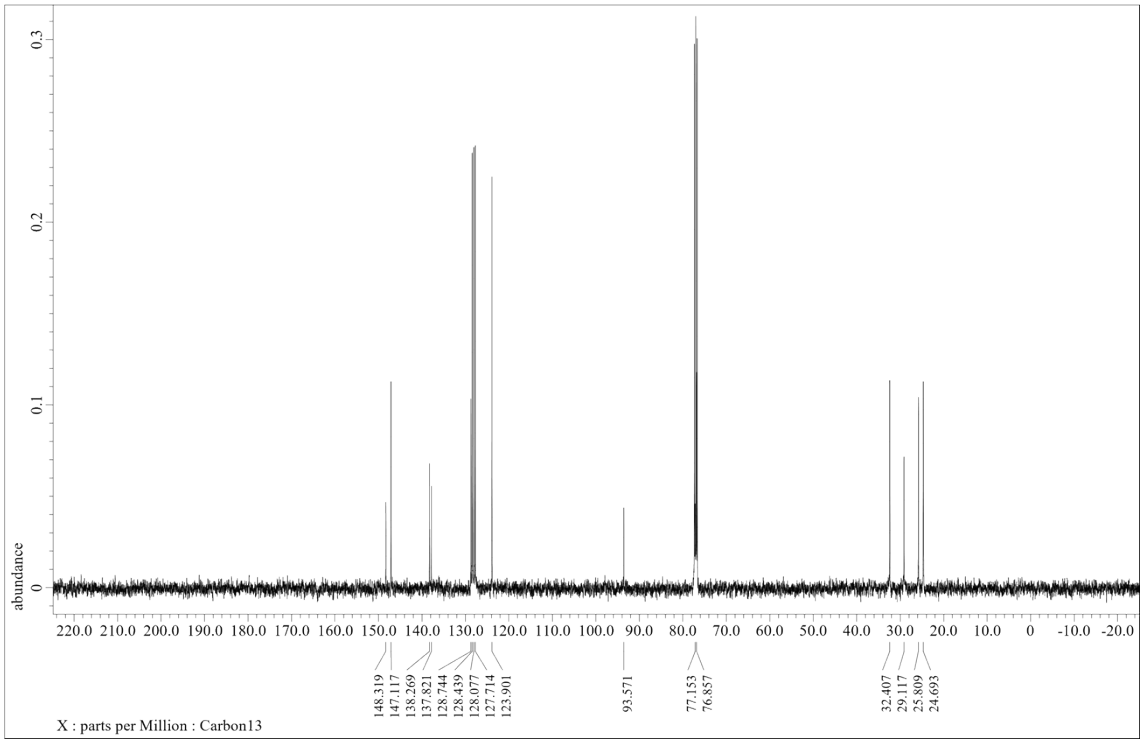
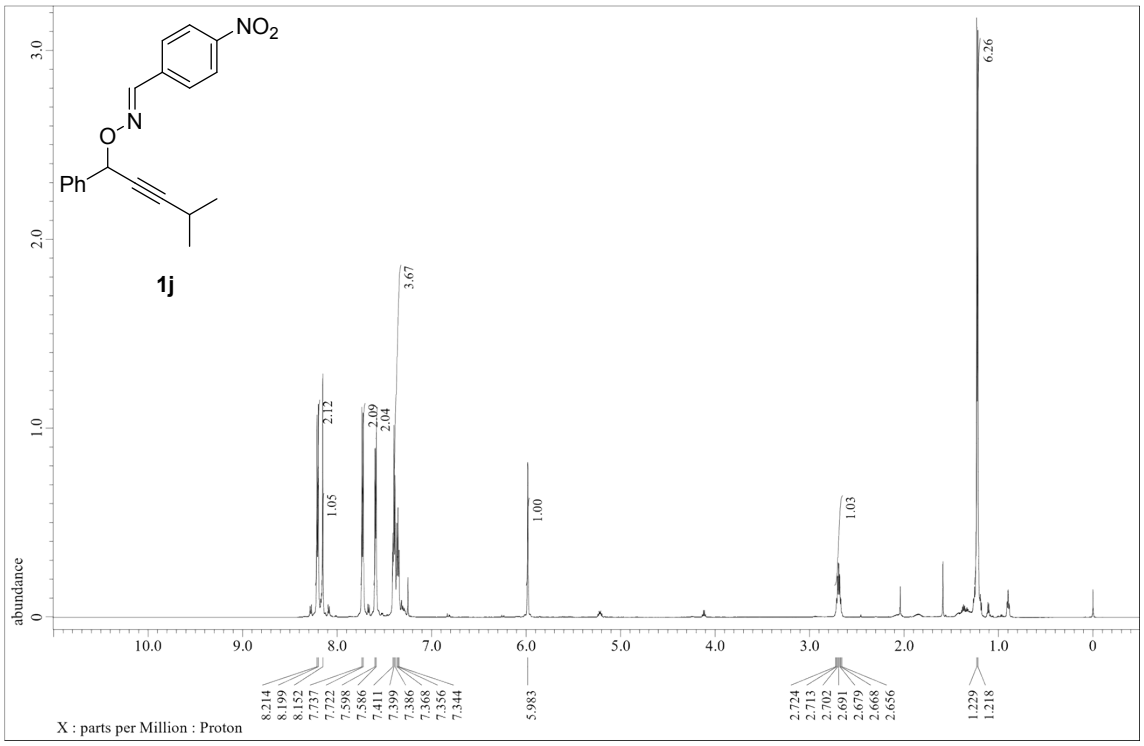
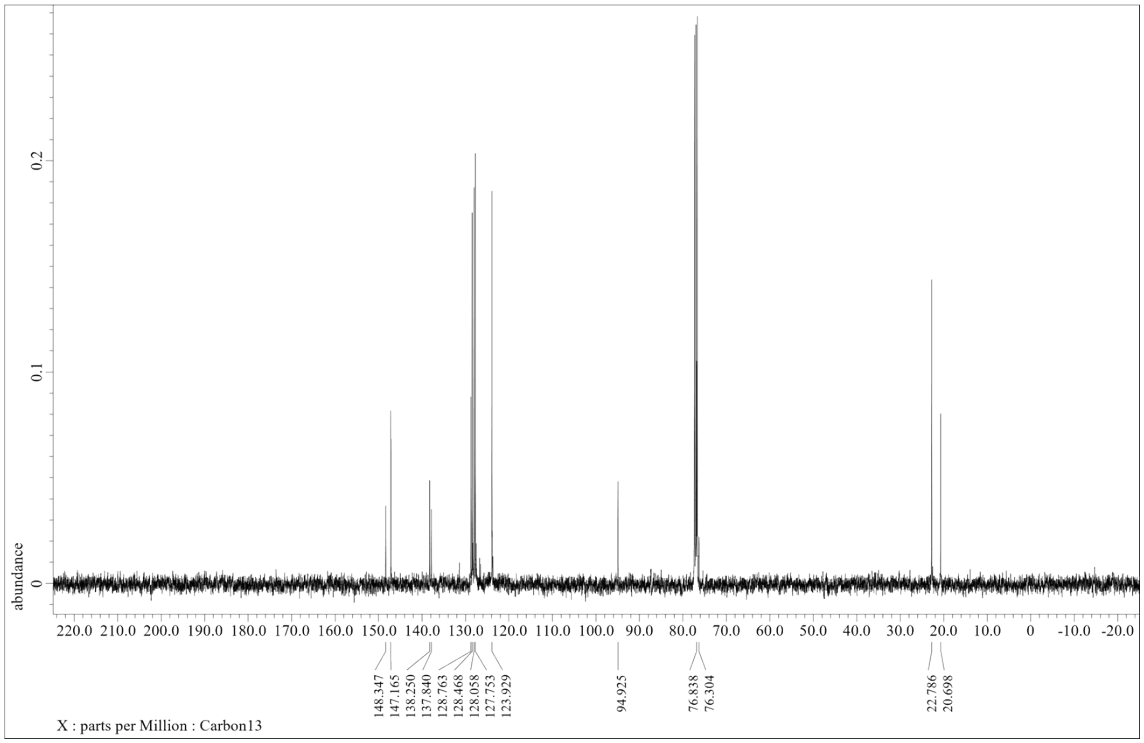
8.213
8.168
7.762
7.740
7.612
7.595
7.426
7.410
7.391
7.367
7.347
6.217
6.097
2.175
2.104
2.096
1.655
1.645
1.627
1.612
1.596
1.581
X : parts per Million : Proton

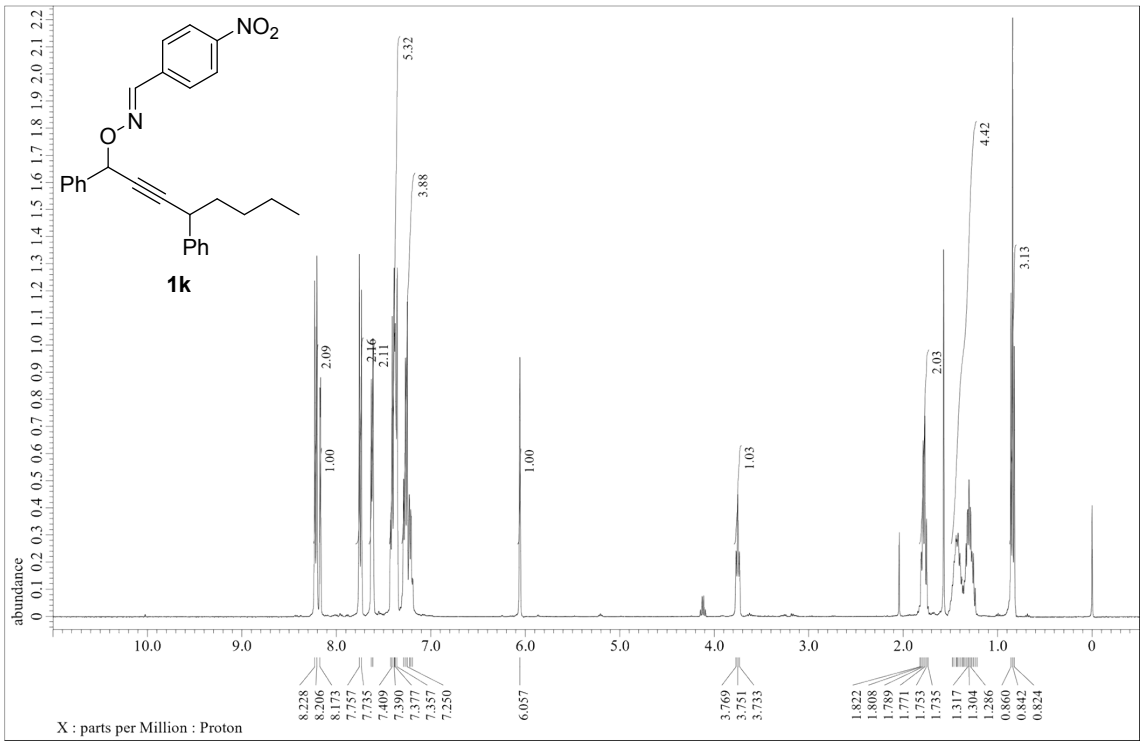

abundance
148.328
147.289
138.183
137.554
136.286
128.811
128.496
128.039
127.762
123.901
119.906
90.215
83.340
77.095
28.974
25.599
22.148
21.347
X : parts per Million : Carbon13

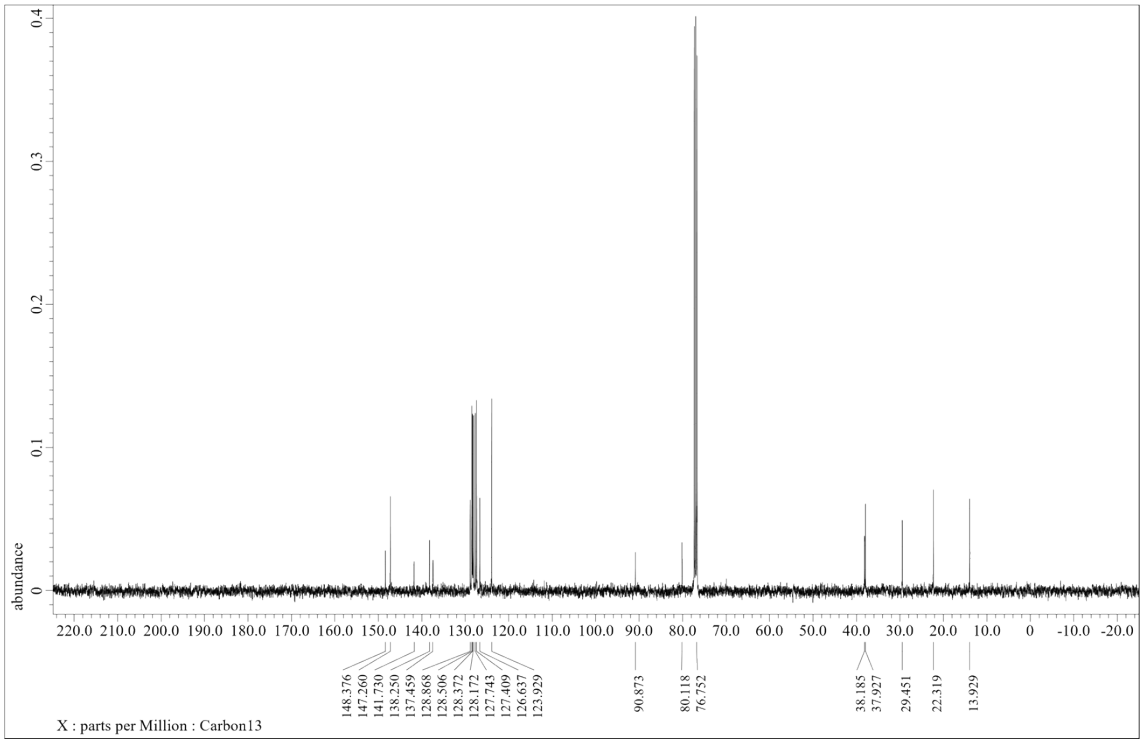

NO2
N
O
Ph
1i
abundance
X : parts per Million : Proton

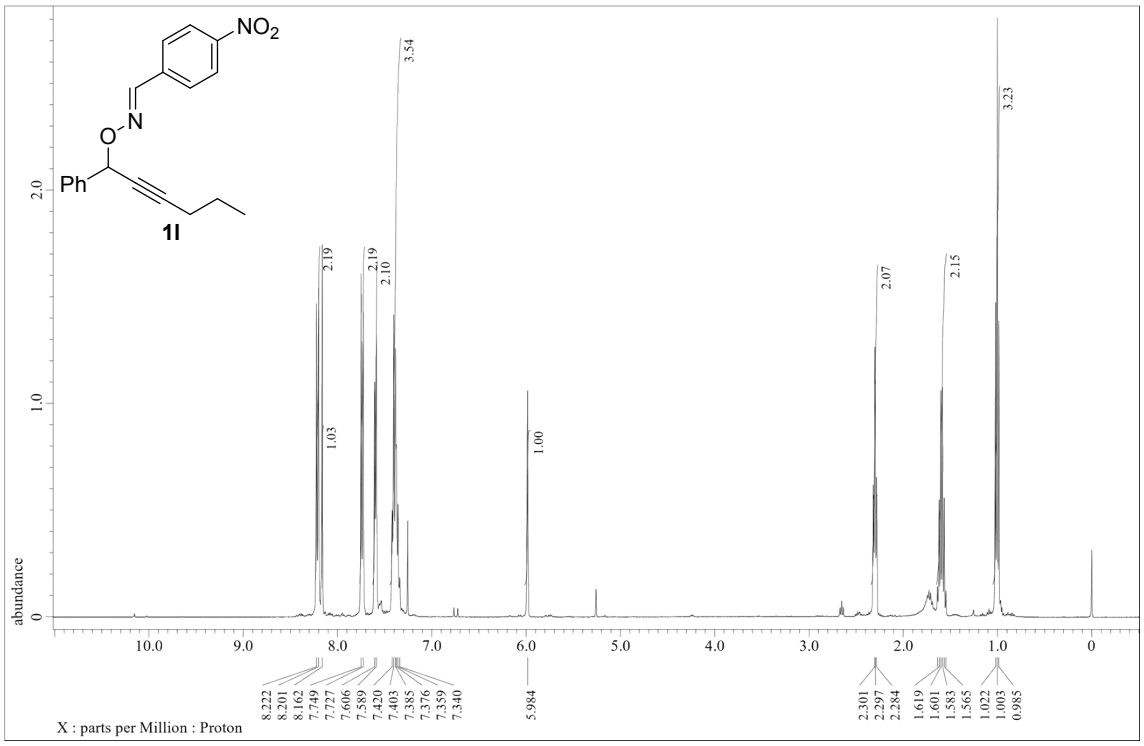

abundance
X : parts per Million : Carbon13

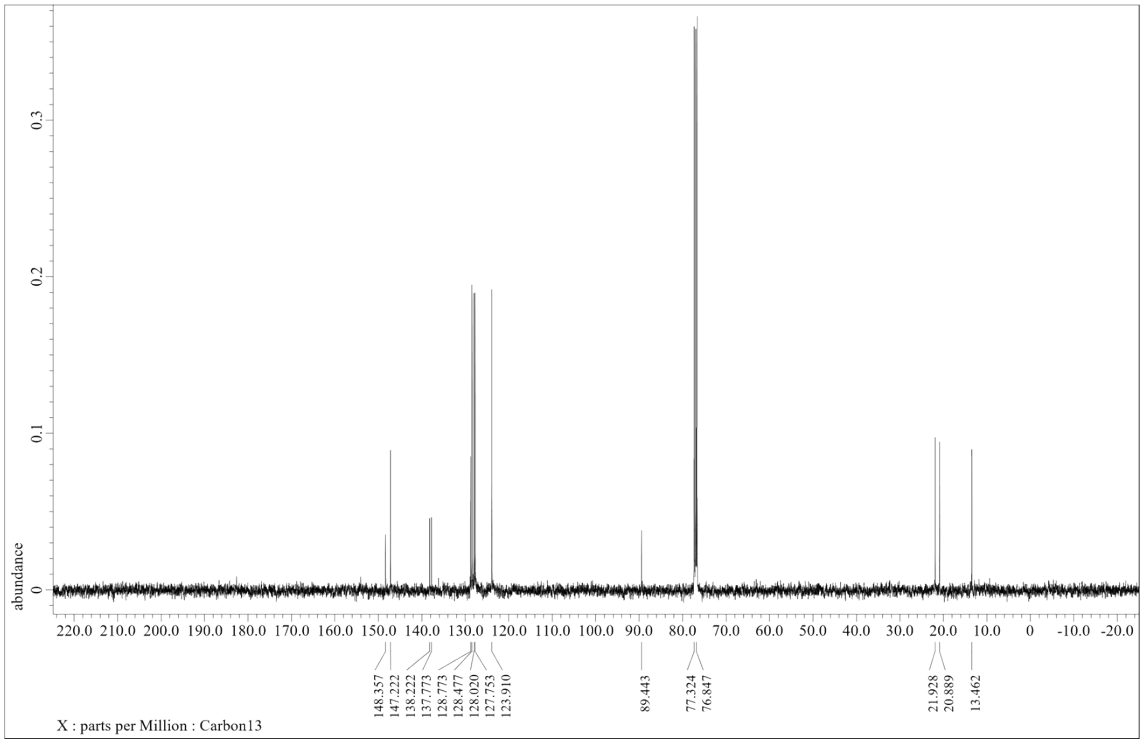

NO2
N
O
Ph
1j
abundance
3.0
2.0
1.0
0
6.26
3.67
2.12
2.09
2.04
1.05
1.00
1.03
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.214
8.199
8.152
7.737
7.722
7.598
7.586
7.411
7.399
7.386
7.368
7.356
7.344
5.983
2.724
2.713
2.702
2.691
2.679
2.668
2.656
1.229
1.218
X : parts per Million : Proton

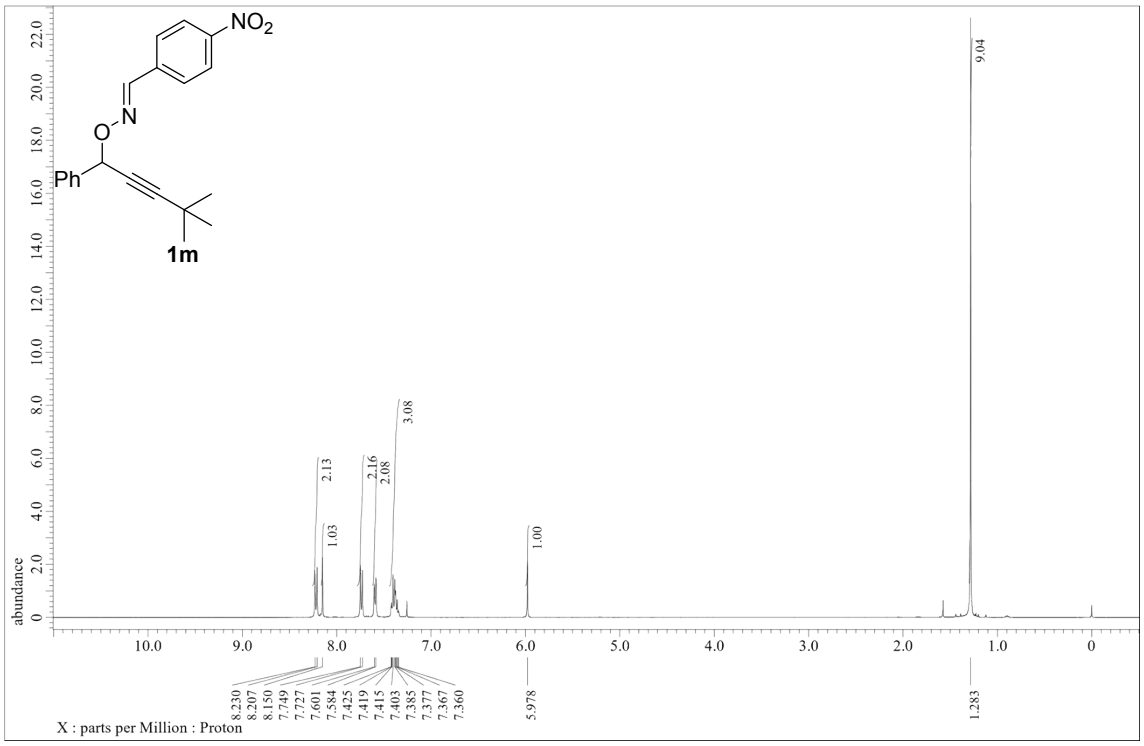

abundance
0.2
0.1
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
148.347
147.165
138.250
137.840
128.763
128.468
128.058
127.753
123.929
94.925
76.838
76.304
22.786
20.698
X : parts per Million : Carbon13

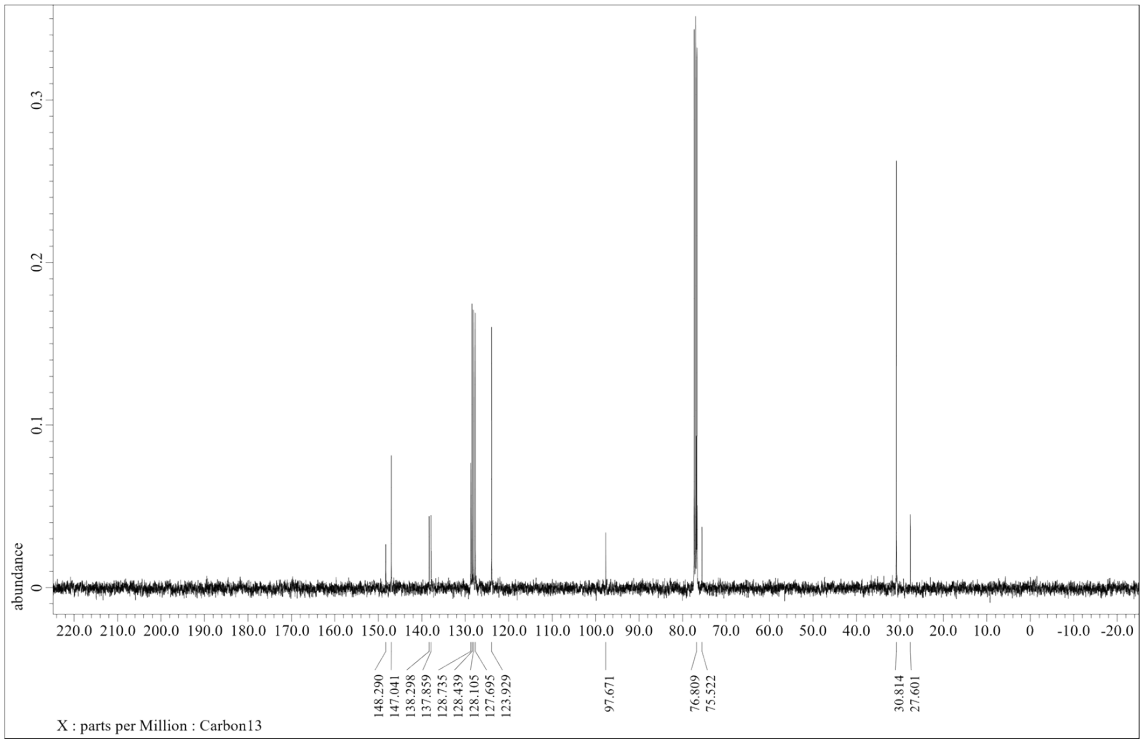

NO2
N
O
Ph
Ph
1k
abundance
X : parts per Million : Proton
5.32
4.42
3.88
3.13
2.09
2.16
2.11
2.03
1.00
1.00
1.03
8.228
8.206
8.173
7.757
7.735
7.409
7.390
7.377
7.357
7.250
6.057
3.769
3.751
3.733
1.822
1.808
1.789
1.771
1.753
1.735
1.317
1.304
1.286
0.860
0.842
0.824

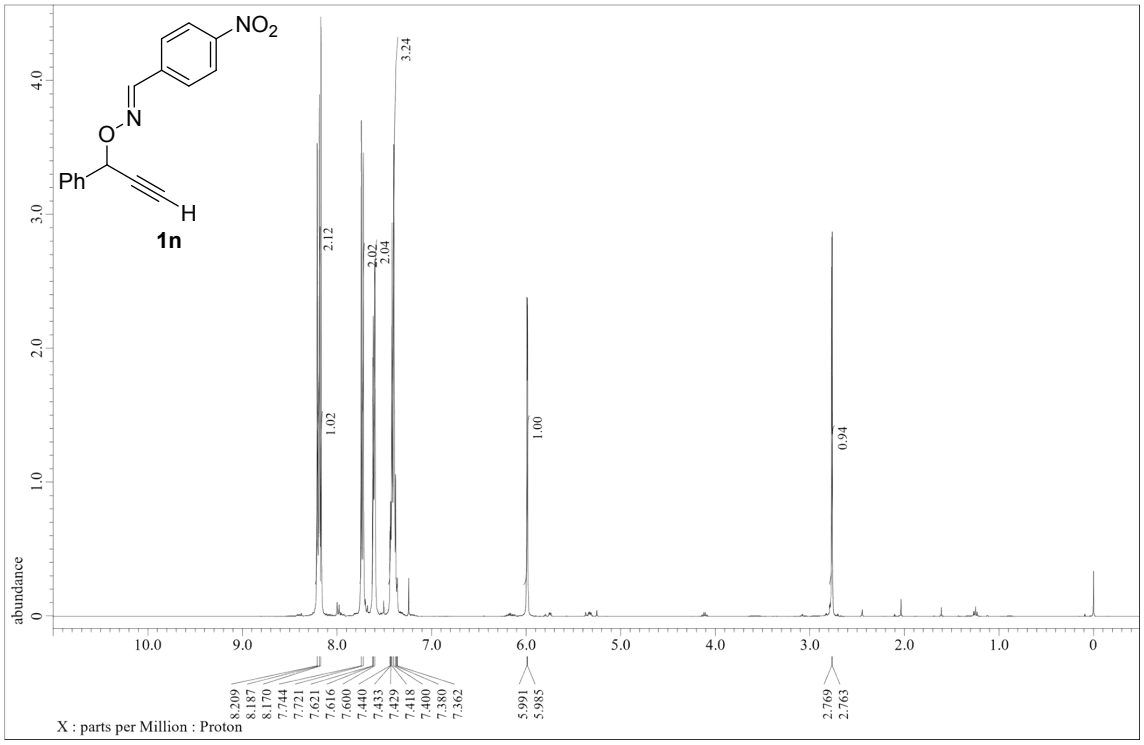

abundance
X : parts per Million : Carbon13
148.376
147.260
141.730
138.250
137.459
128.868
128.506
128.372
128.172
127.743
127.409
126.637
123.929
90.873
80.118
76.752
38.185
37.927
29.451
22.319
13.929

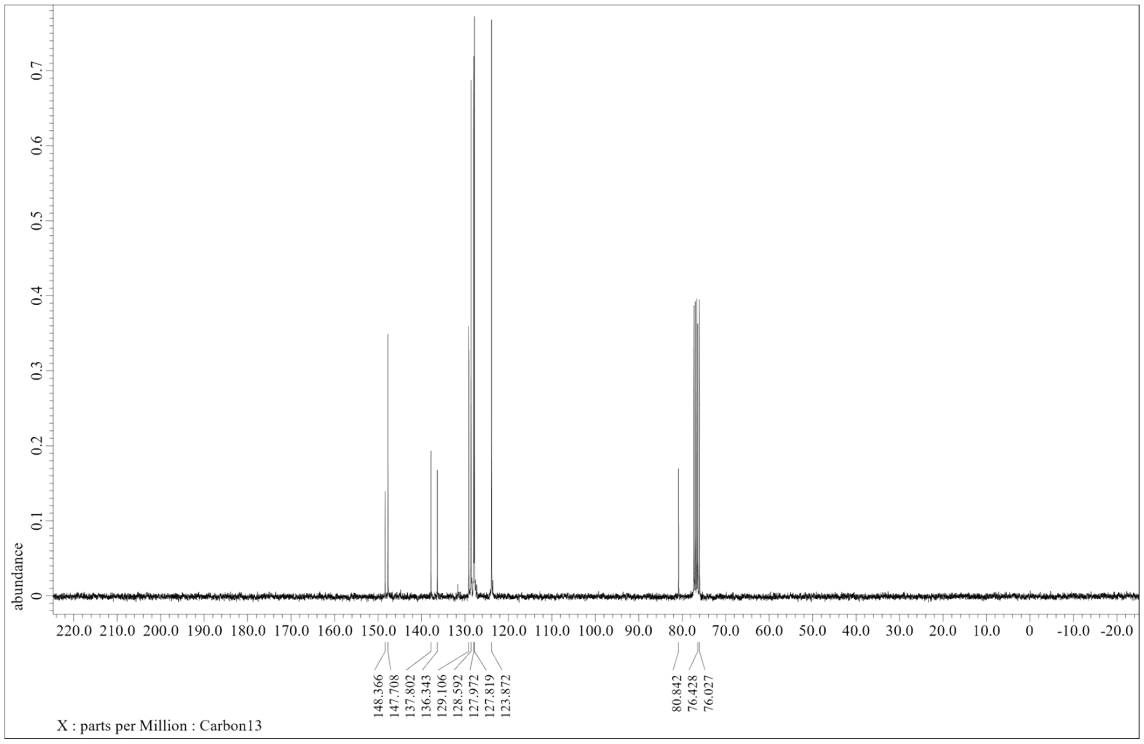

NO2
N
O
Ph
1l
abundance
2.0
1.0
0
3.54
3.23
2.19
2.19
2.10
2.07
2.15
1.03
1.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.222
8.201
8.162
7.749
7.727
7.606
7.589
7.420
7.403
7.385
7.376
7.359
7.340
5.984
2.301
2.297
2.284
1.619
1.601
1.583
1.565
1.022
1.003
0.985
X : parts per Million : Proton

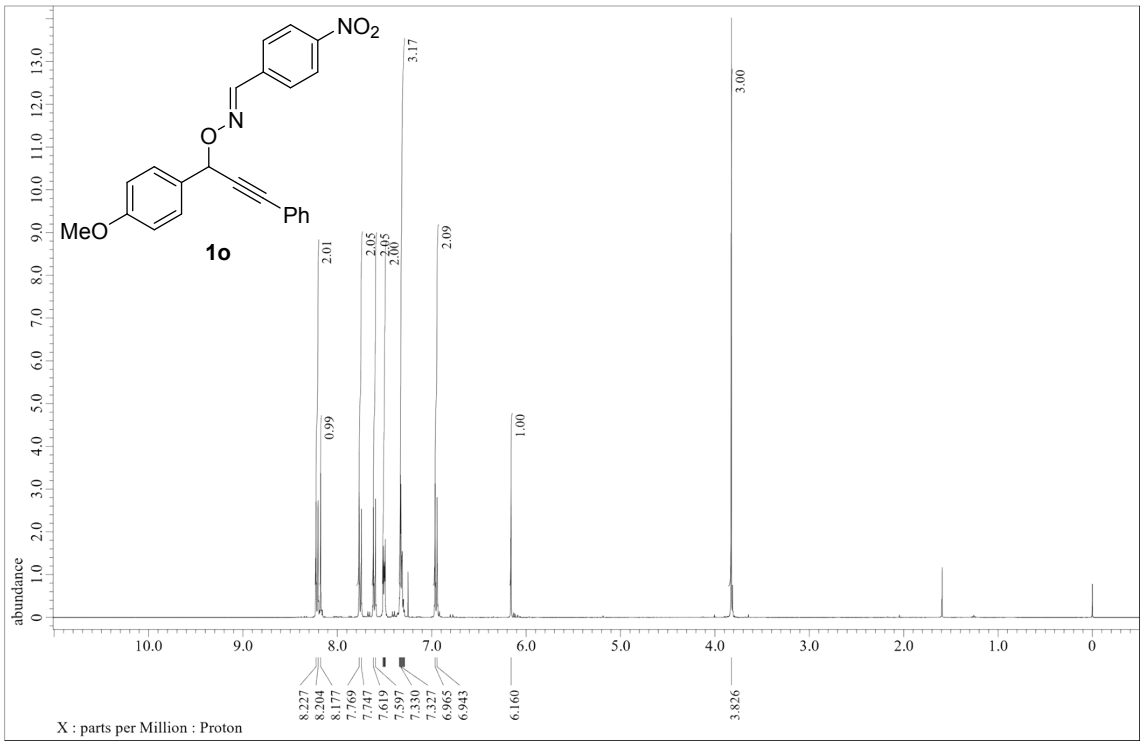

abundance
0.3
0.2
0.1
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
148.357
147.222
138.222
137.773
128.773
128.477
128.020
127.753
123.910
89.443
77.324
76.847
21.928
20.889
13.462
X : parts per Million : Carbon13

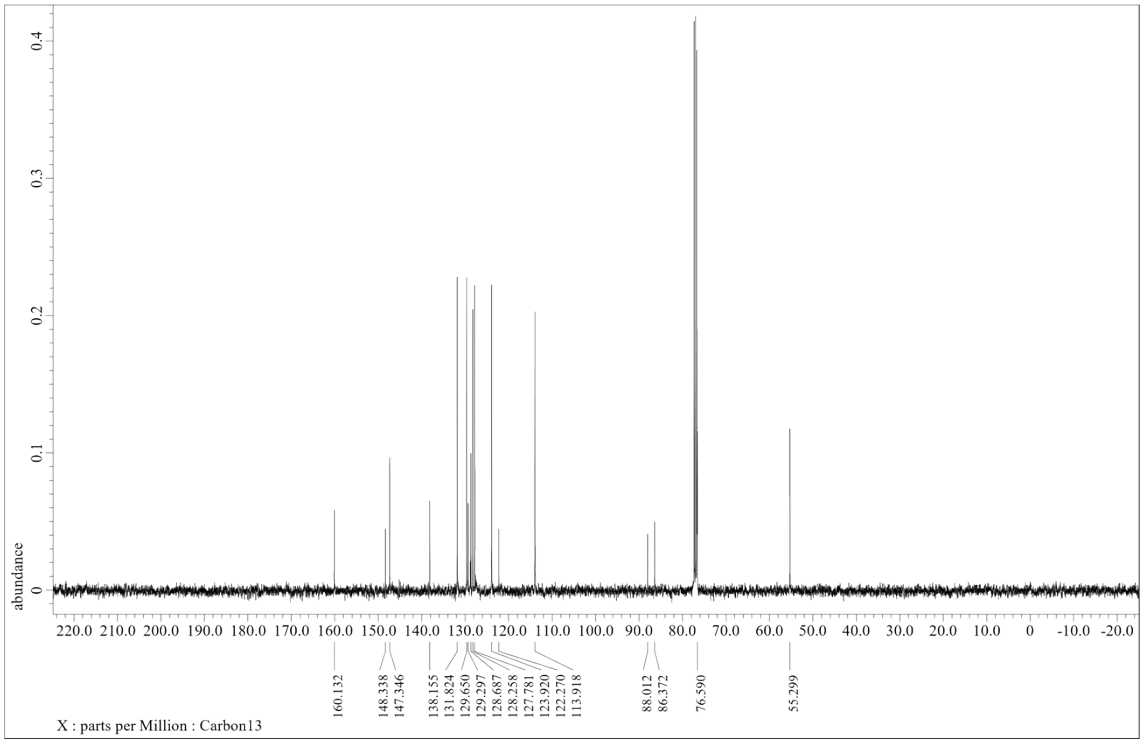

NO2
N
O
Ph
1m
abundance
9.04
3.08
2.13
2.16
2.08
1.03
1.00
8.230
8.207
8.150
7.749
7.727
7.601
7.584
7.425
7.419
7.415
7.403
7.385
7.377
7.367
7.360
5.978
1.283
X : parts per Million : Proton

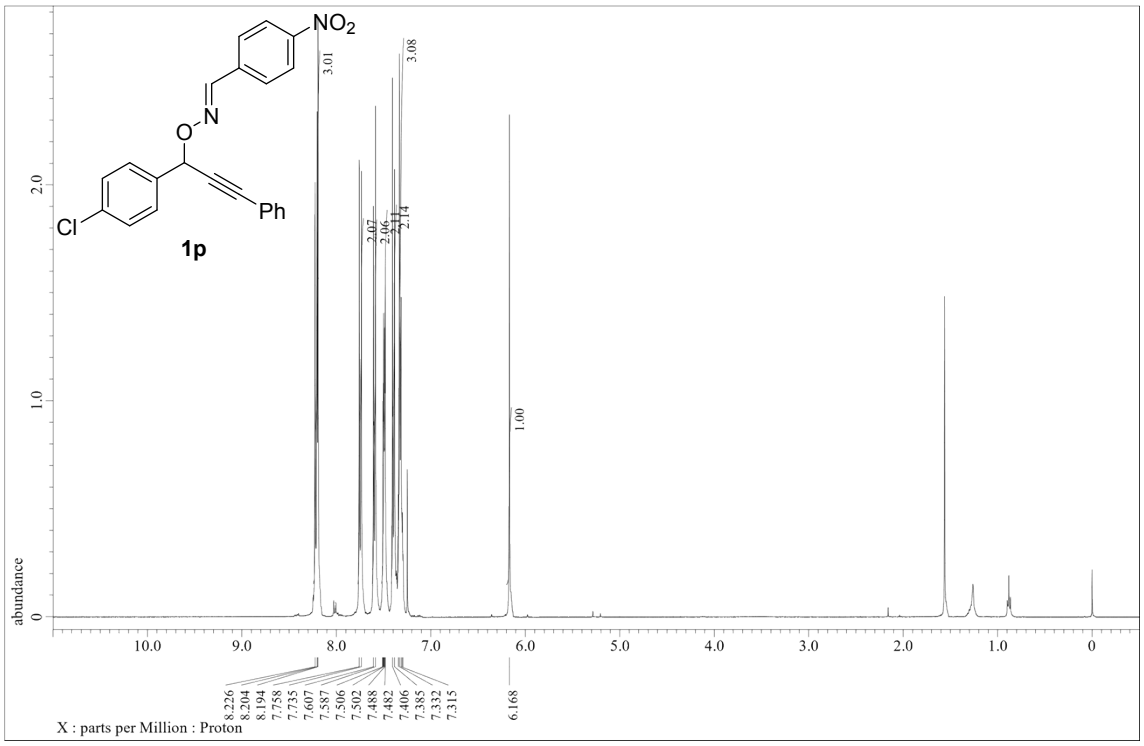

abundance
148.290
147.041
138.298
137.859
128.735
128.439
128.105
127.695
123.929
97.671
76.809
75.522
30.814
27.601
X : parts per Million : Carbon13

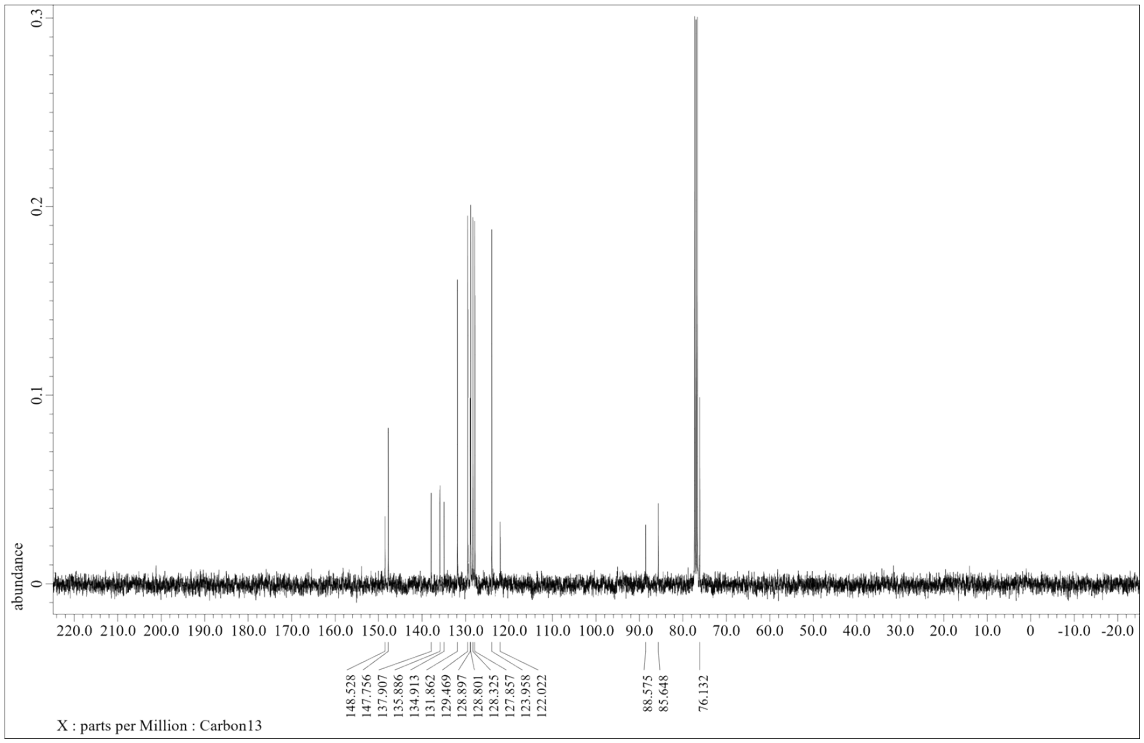

NO2
N
O
Ph
H
1n
3.24
2.12
2.02
2.04
1.02
1.00
0.94
abundance
8.209
8.187
8.170
7.744
7.721
7.621
7.616
7.600
7.440
7.433
7.429
7.418
7.400
7.380
7.362
5.991
5.985
2.769
2.763
X : parts per Million : Proton

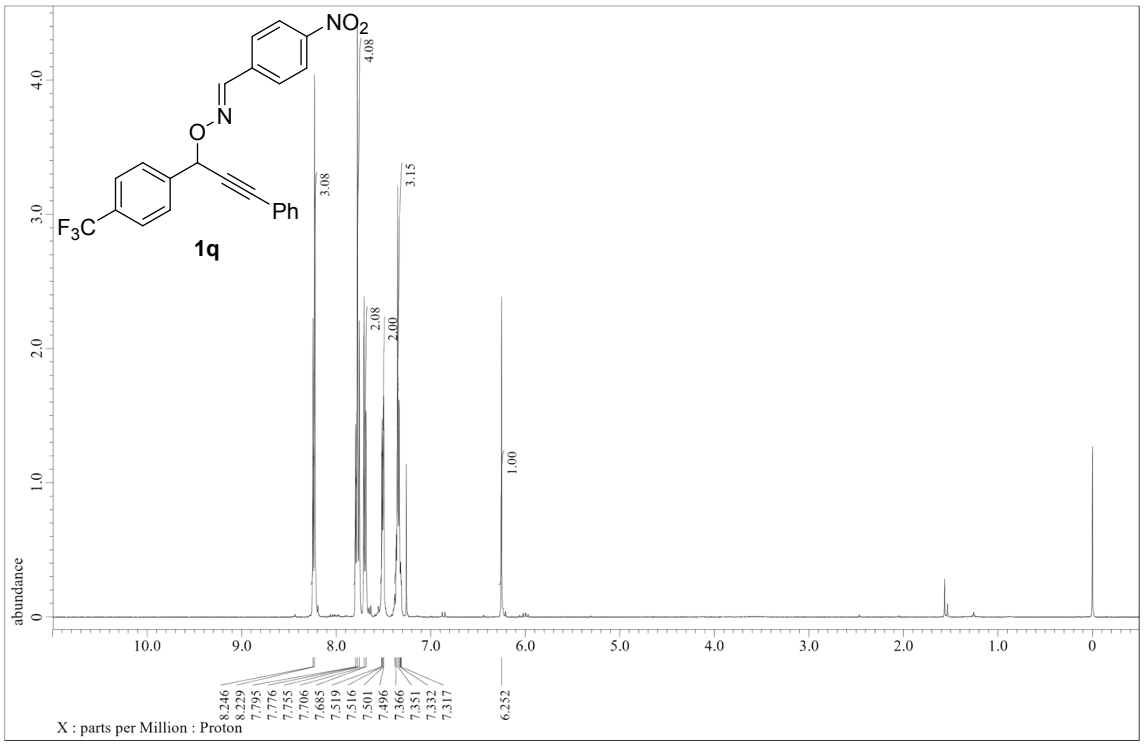

abundance
148.366
147.708
137.802
136.343
129.106
128.592
127.972
127.819
123.872
80.842
76.428
76.027
X : parts per Million : Carbon13

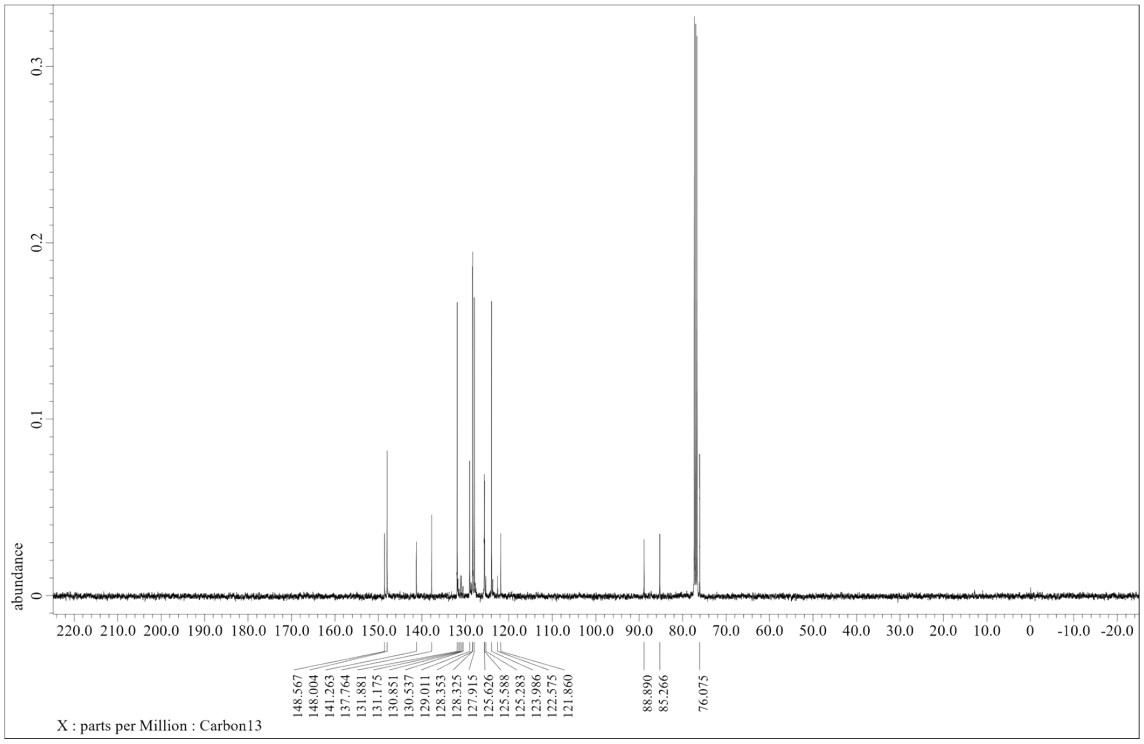

NO2
N
O
MeO
Ph
1o
abundance
X : parts per Million : Proton
8.227
8.204
8.177
7.769
7.747
7.619
7.597
7.330
7.327
6.965
6.943
6.160
3.826

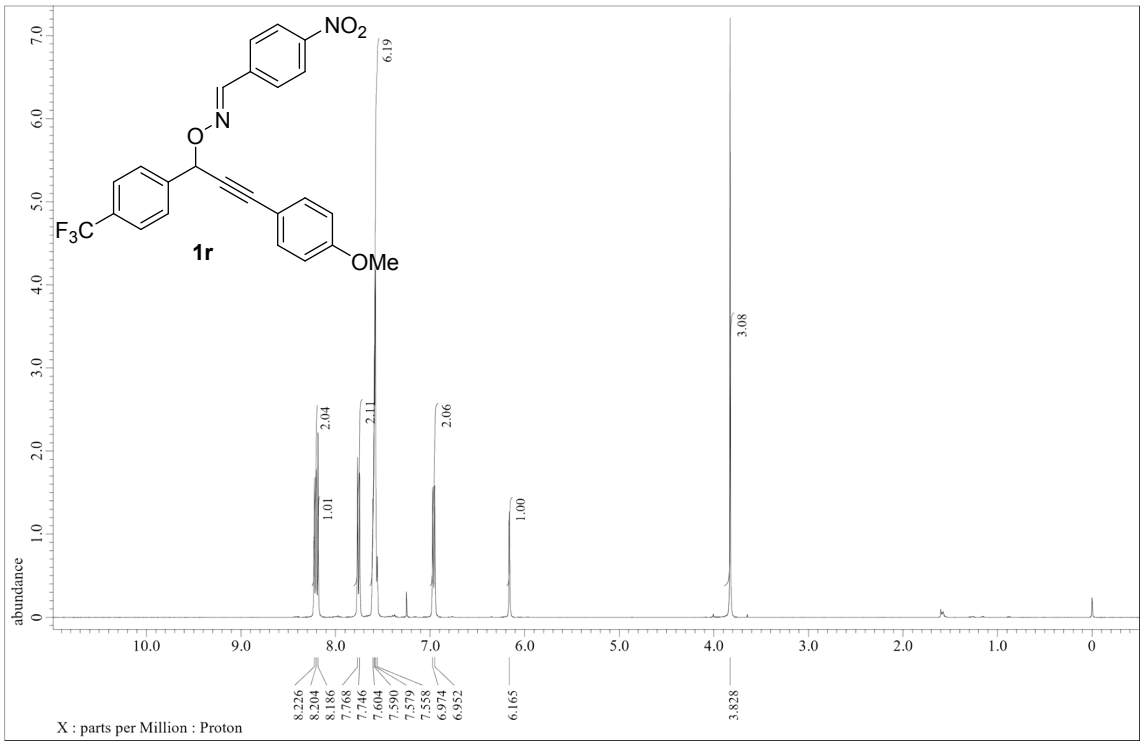

abundance
X : parts per Million : Carbon13
160.132
148.338
147.346
138.155
131.824
129.650
129.297
128.687
128.258
127.781
123.920
122.270
113.918
88.012
86.372
76.590
55.299

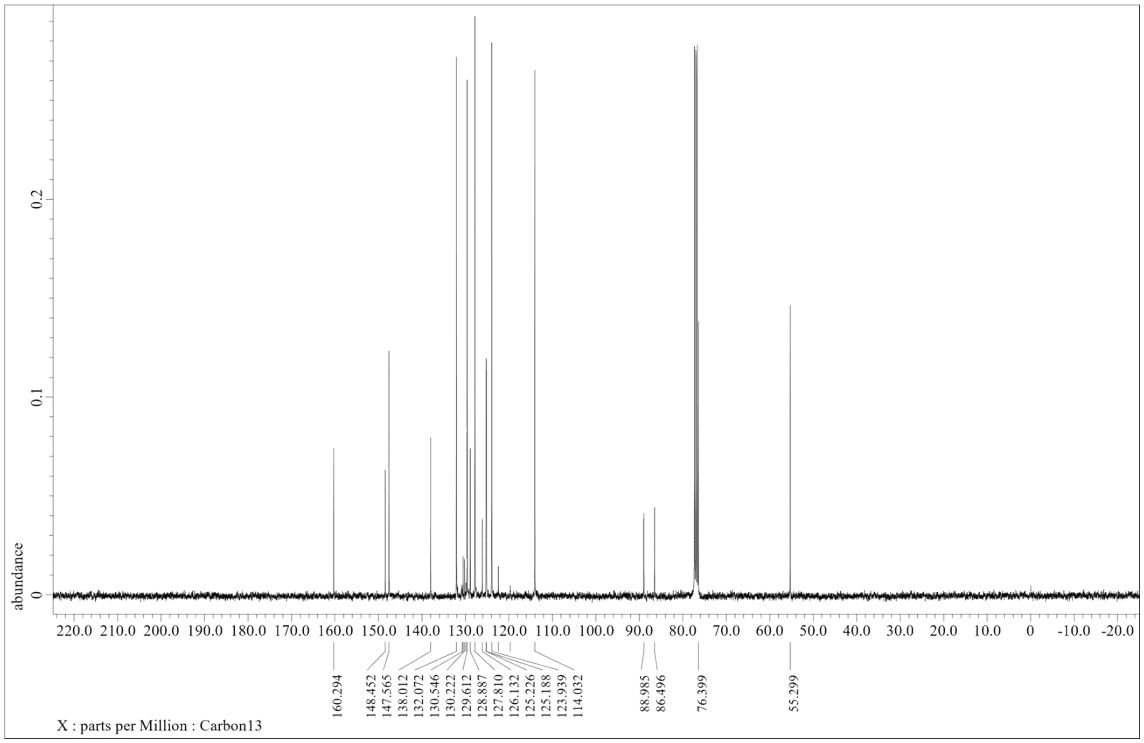

NO2
N
O
Cl
Ph
1p
3.01
3.08
2.07
2.06
2.11
2.14
1.00
abundance
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.226
8.204
8.194
7.758
7.735
7.607
7.587
7.506
7.502
7.488
7.482
7.406
7.385
7.332
7.315
6.168
X : parts per Million : Proton

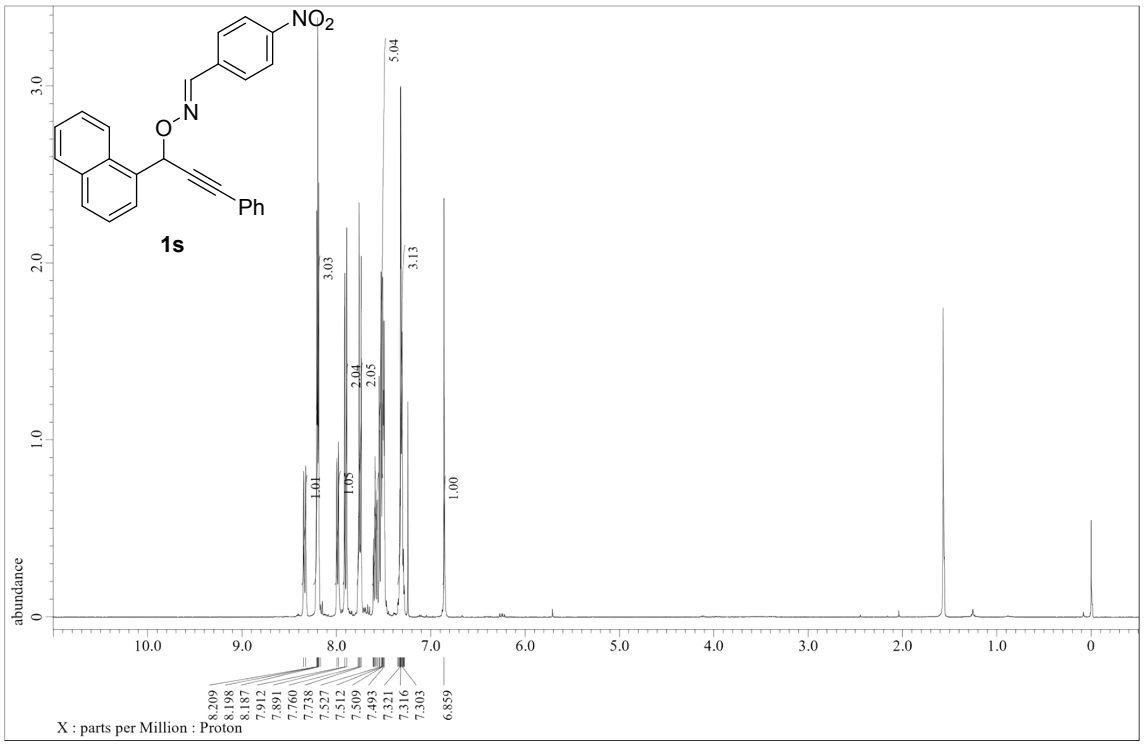

abundance
0.3
0.2
0.1
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
148.528
147.756
137.907
135.886
134.913
131.862
129.469
128.897
128.801
128.325
127.857
123.958
122.022
88.575
85.648
76.132
X : parts per Million : Carbon13

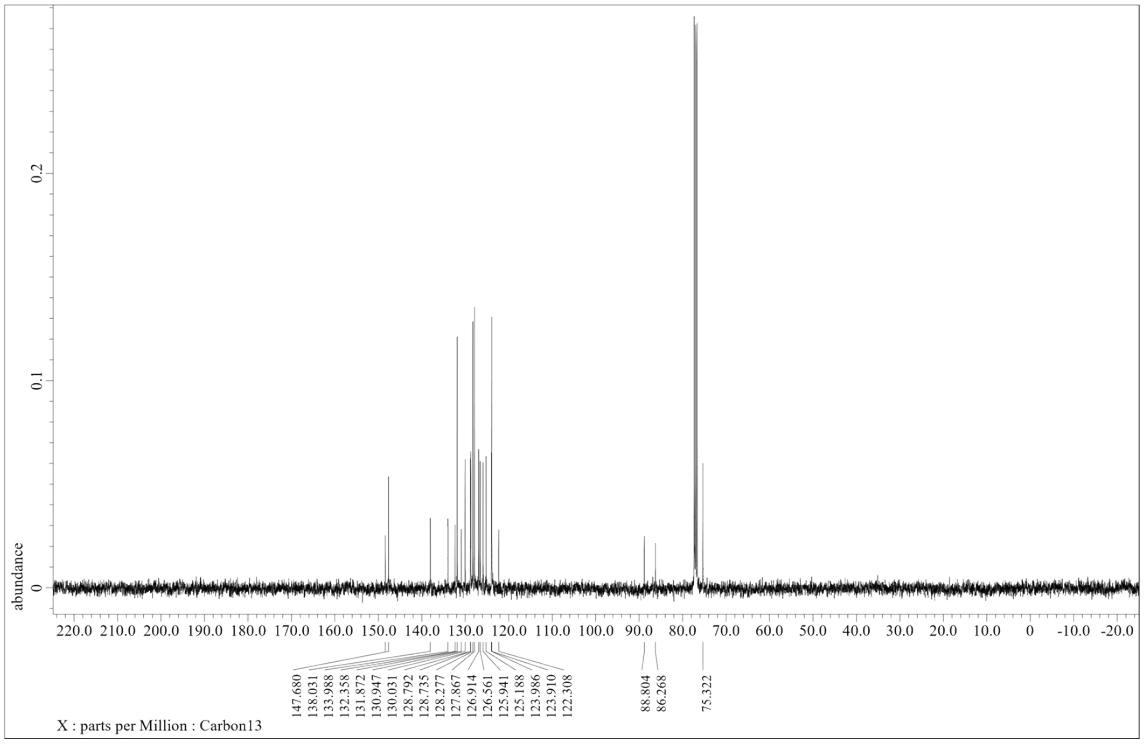

NO2
N
O
F3C
Ph
1q
4.08
3.08
3.15
2.08
2.00
1.00
abundance
8.246
8.229
7.795
7.776
7.755
7.706
7.685
7.519
7.516
7.501
7.496
7.366
7.351
7.332
7.317
6.252
X : parts per Million : Proton

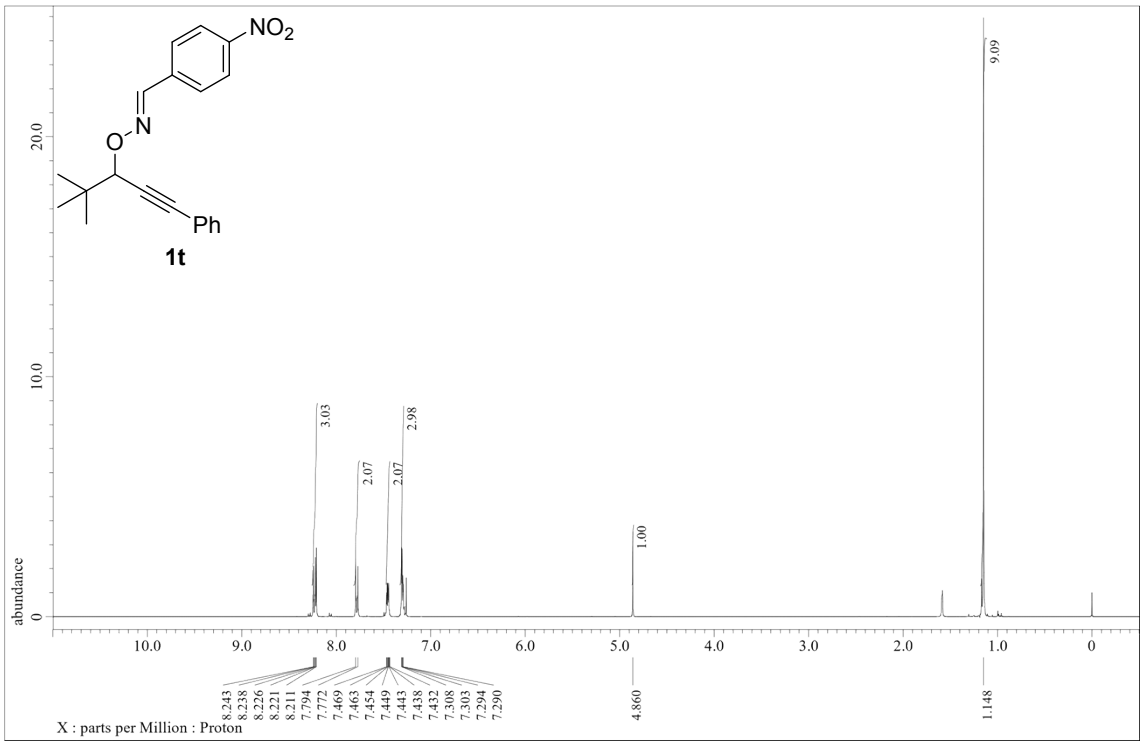

abundance
148.567
148.004
141.263
137.764
131.881
131.175
130.851
130.537
129.011
128.353
128.325
127.915
125.626
125.588
125.283
123.986
122.575
121.860
88.890
85.266
76.075
X : parts per Million : Carbon13

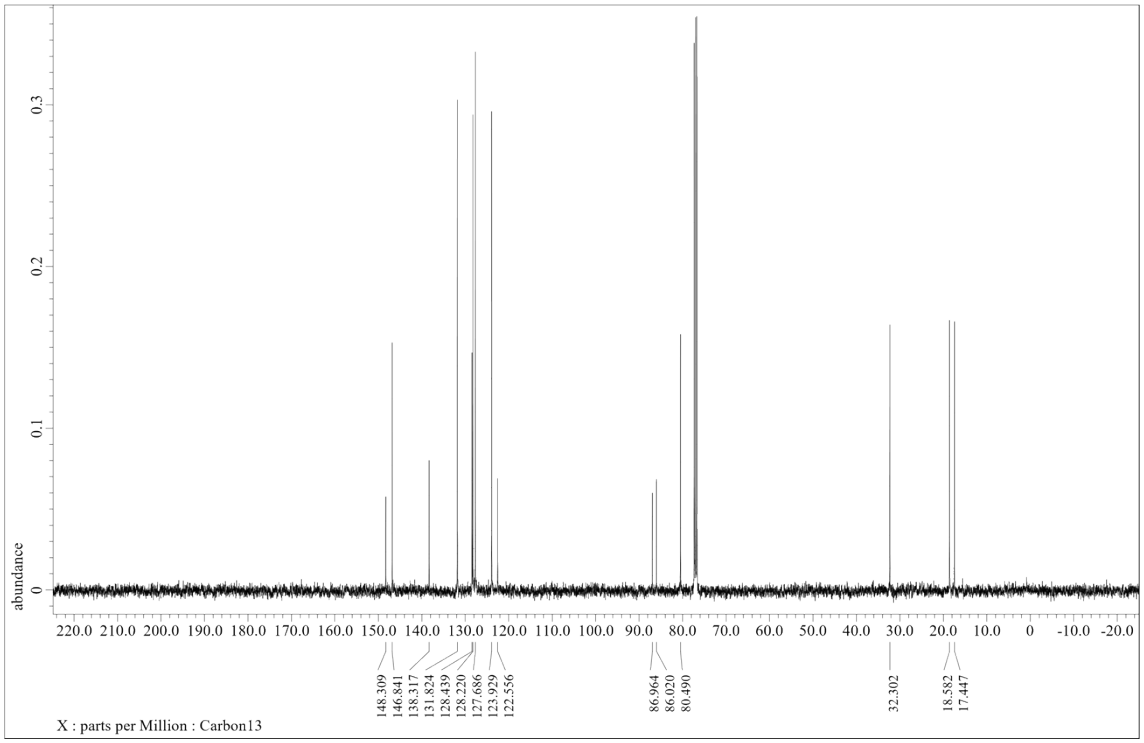

NO2
N
O
F3C
OMe
1r
6.19
3.08
2.04
2.11
2.06
1.01
1.00
abundance
X : parts per Million : Proton
8.226
8.204
8.186
7.768
7.746
7.604
7.590
7.579
7.558
6.974
6.952
6.165
3.828

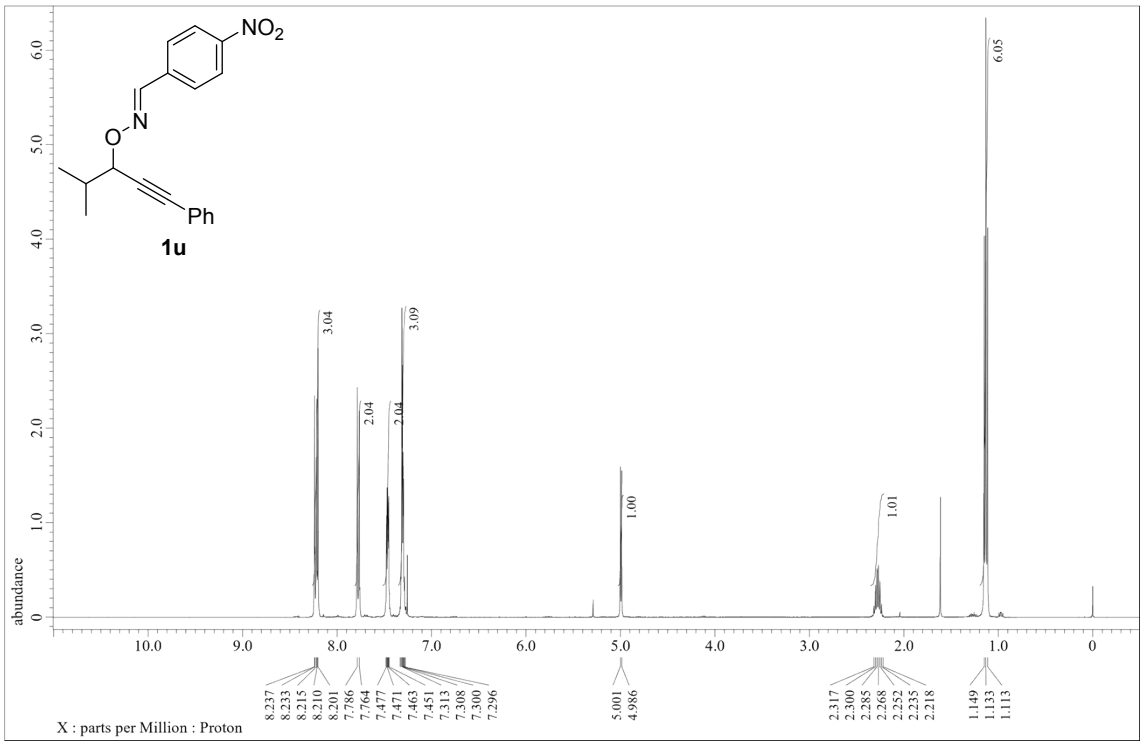

abundance
X : parts per Million : Carbon13
160.294
148.452
147.565
138.012
132.072
130.546
130.222
129.612
128.887
127.810
126.132
125.226
125.188
123.939
114.032
88.985
86.496
76.399
55.299

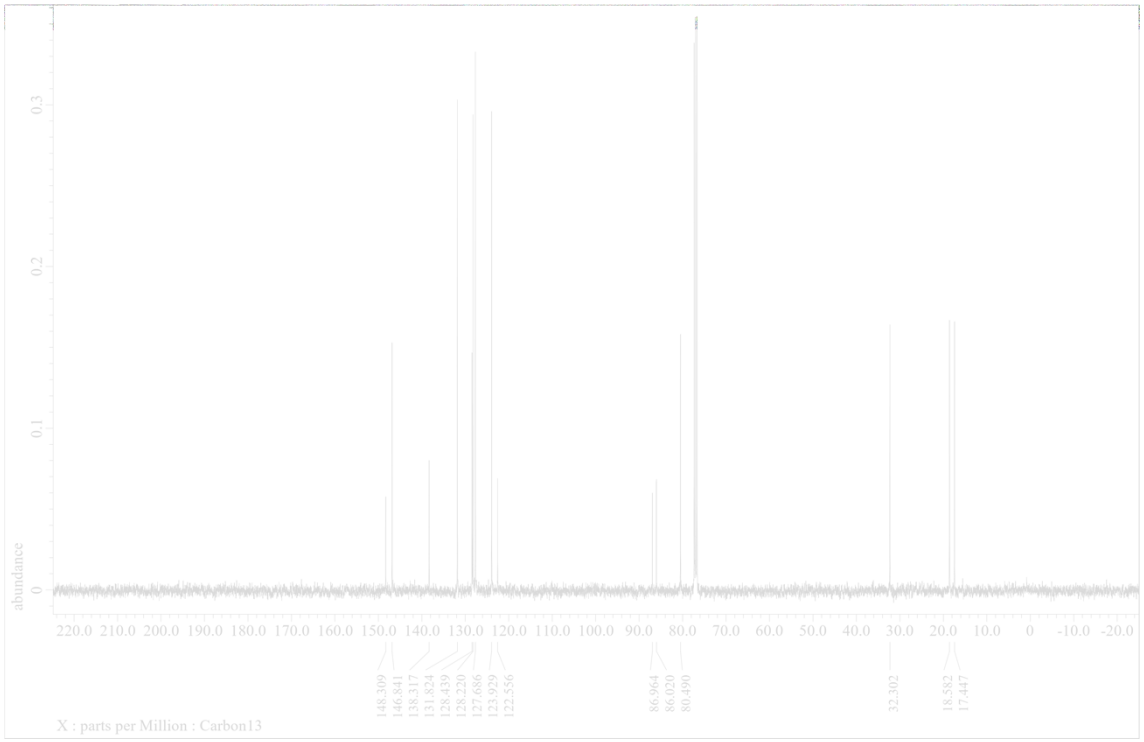

NO2
N
O
Ph
1s
5.04
3.03
3.13
2.04
2.05
1.01
1.05
1.00
abundance
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.209
8.198
8.187
7.912
7.891
7.760
7.738
7.527
7.512
7.509
7.493
7.321
7.316
7.303
6.859
X : parts per Million : Proton

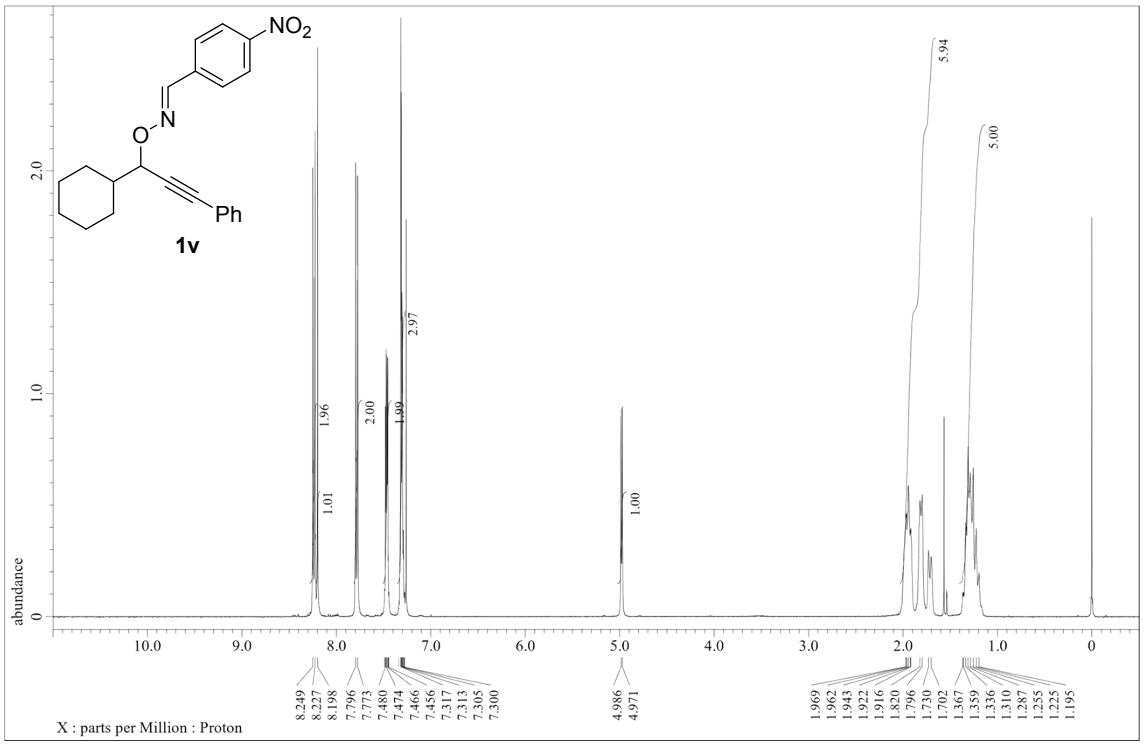

abundance
0.2
0.1
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
147.680
138.031
133.988
132.358
131.872
130.947
130.031
128.792
128.735
128.277
127.867
126.914
126.561
125.941
125.188
123.986
123.910
122.308
88.804
86.268
75.322
X : parts per Million : Carbon13

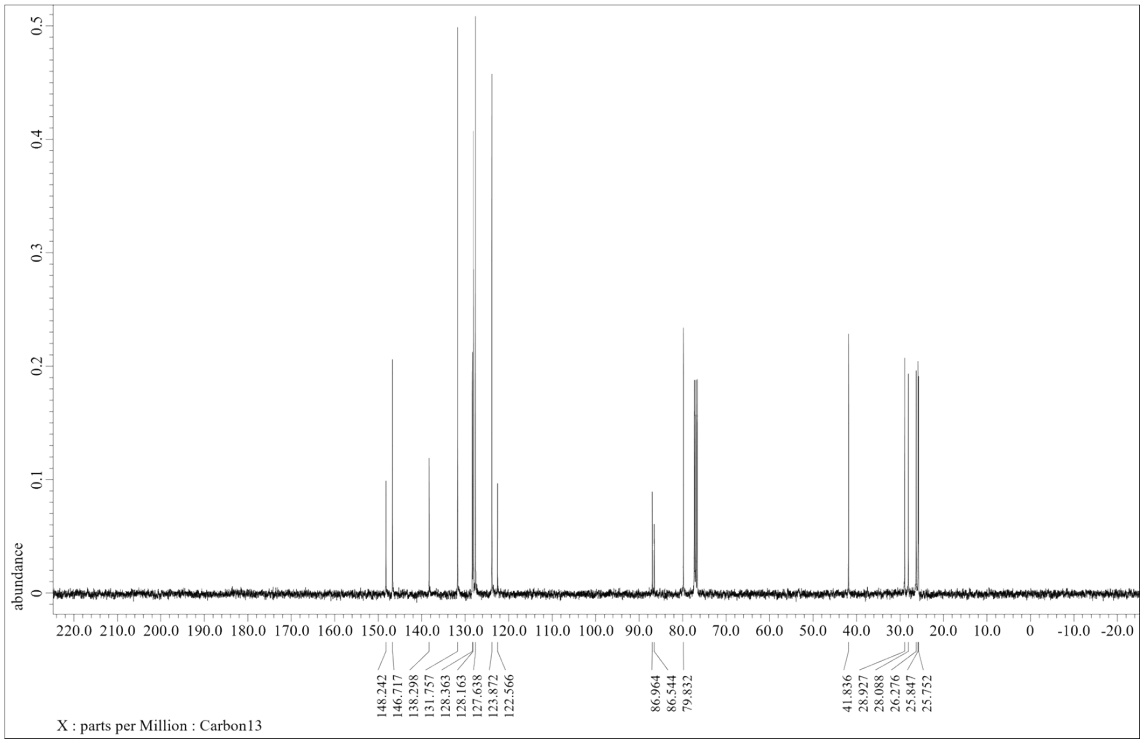

NO2
N
O
Ph
1t
abundance
20.0
10.0
0
3.03
2.07
2.07
2.98
1.00
9.09
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
8.243
8.238
8.226
8.221
8.211
7.794
7.772
7.469
7.463
7.454
7.449
7.443
7.438
7.432
7.308
7.303
7.294
7.290
4.860
1.148
X : parts per Million : Proton

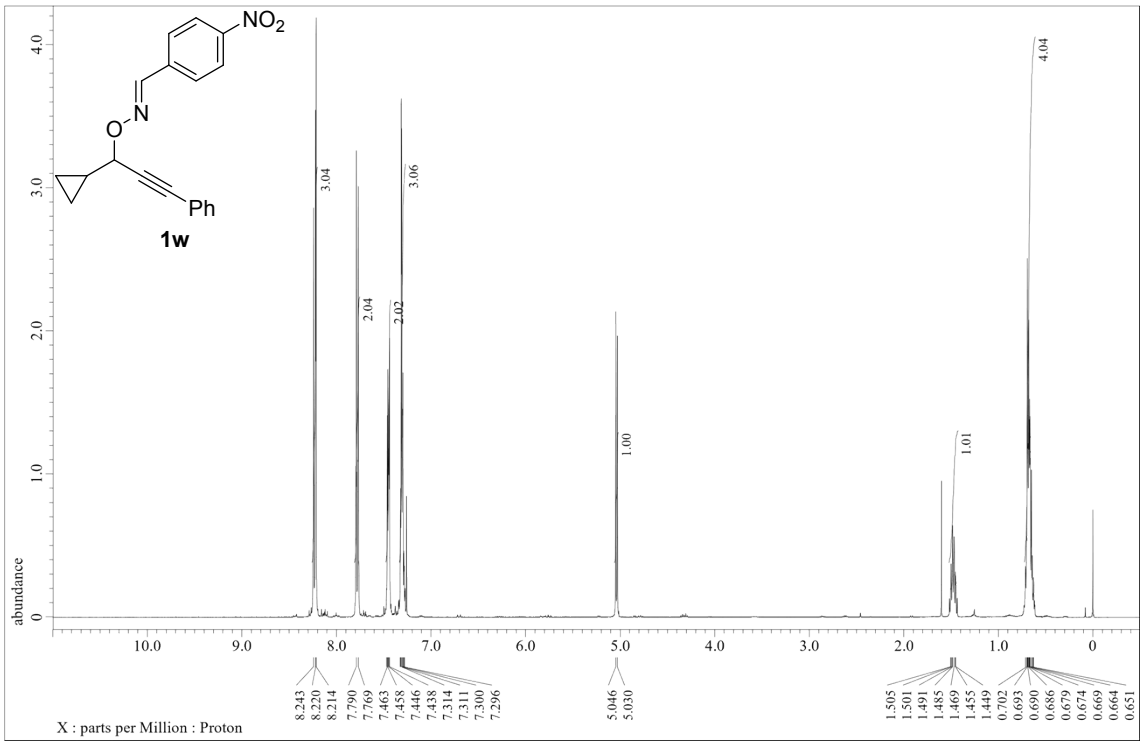

abundance
0.3
0.2
0.1
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
148.309
146.841
138.317
131.824
128.439
128.220
127.686
123.929
122.556
86.964
86.020
80.490
32.302
18.582
17.447
X : parts per Million : Carbon13

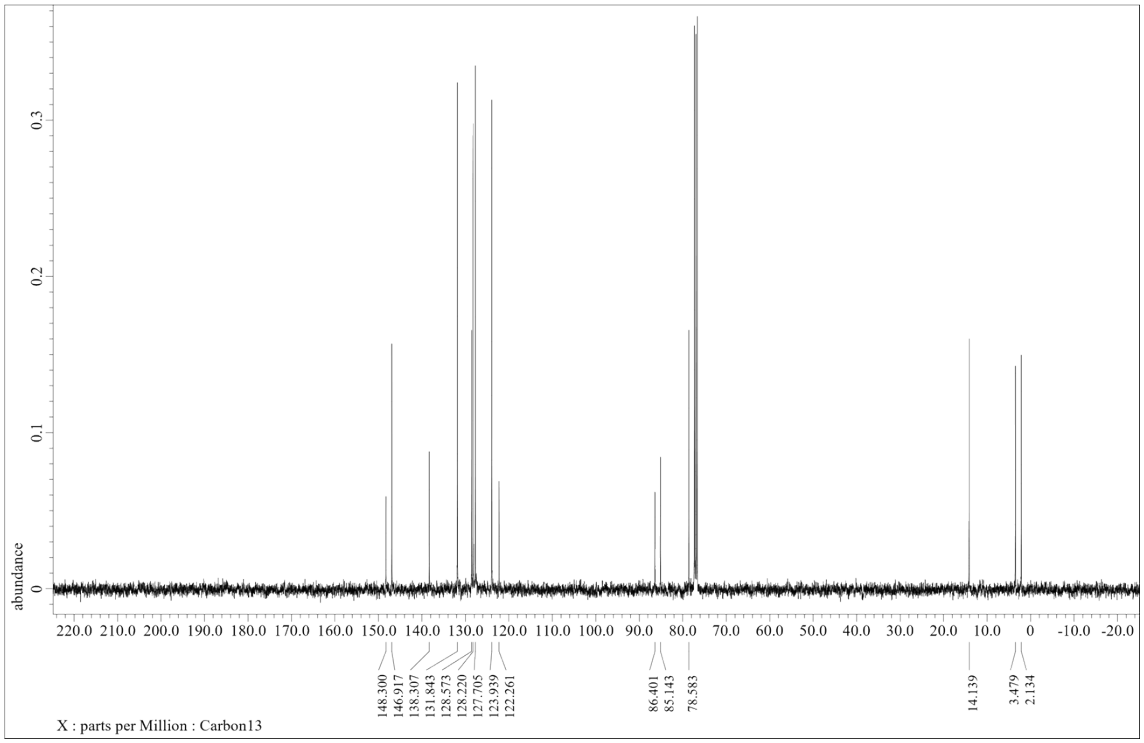

NO2
N
O
Ph
1u
abundance
X : parts per Million : Proton

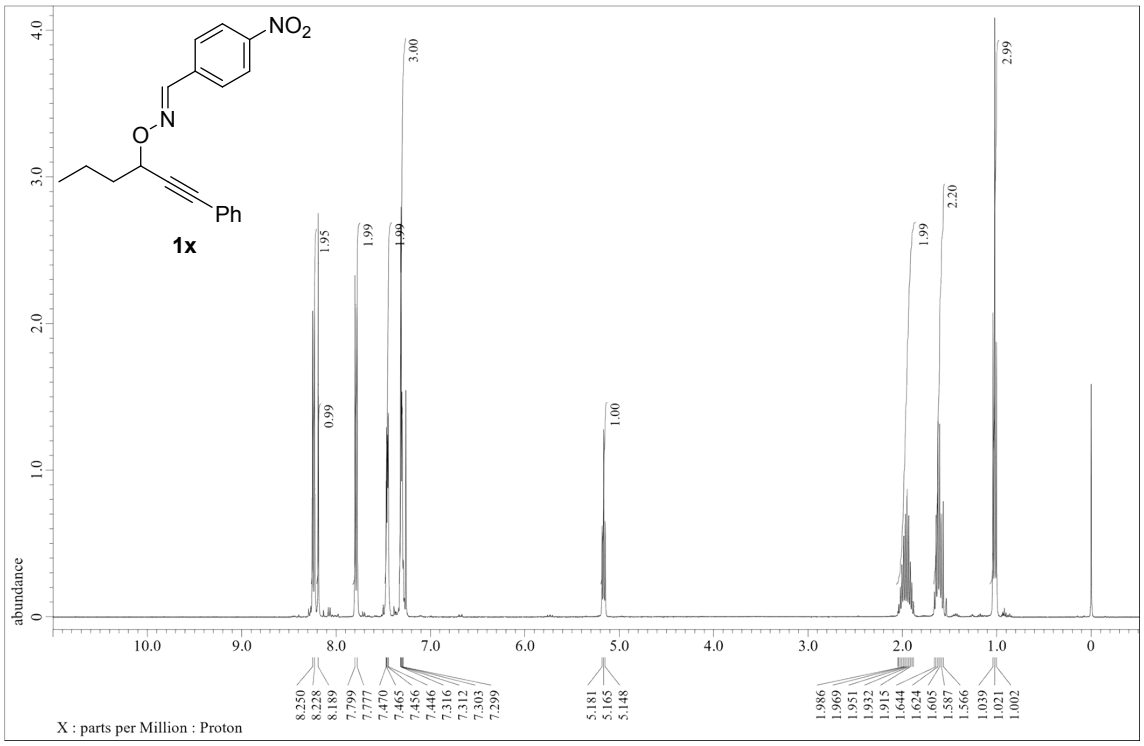

abundance
X : parts per Million : Carbon13

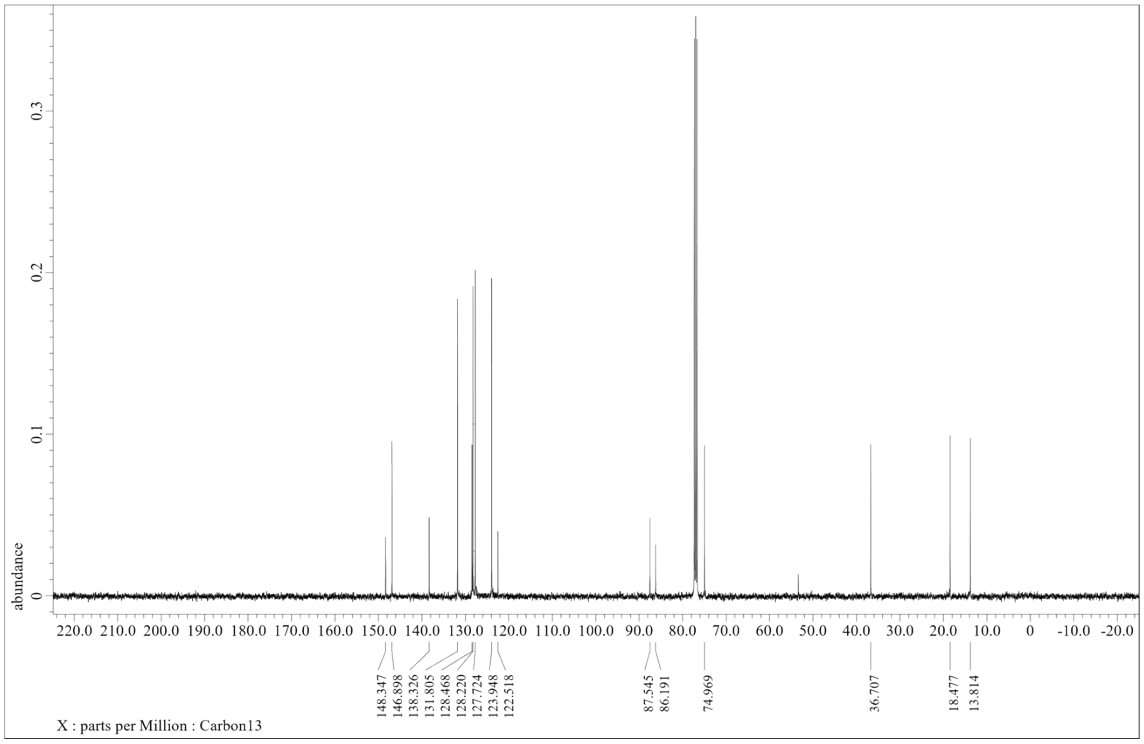

NO2
N
O
Ph
1v
abundance
2.0
1.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.01
1.96
2.00
1.09
2.97
1.00
5.94
5.00
8.249
8.227
8.198
7.796
7.773
7.480
7.474
7.466
7.456
7.317
7.313
7.305
7.300
4.986
4.971
1.969
1.962
1.943
1.922
1.916
1.820
1.796
1.730
1.702
1.367
1.359
1.336
1.310
1.287
1.255
1.225
1.195
X : parts per Million : Proton

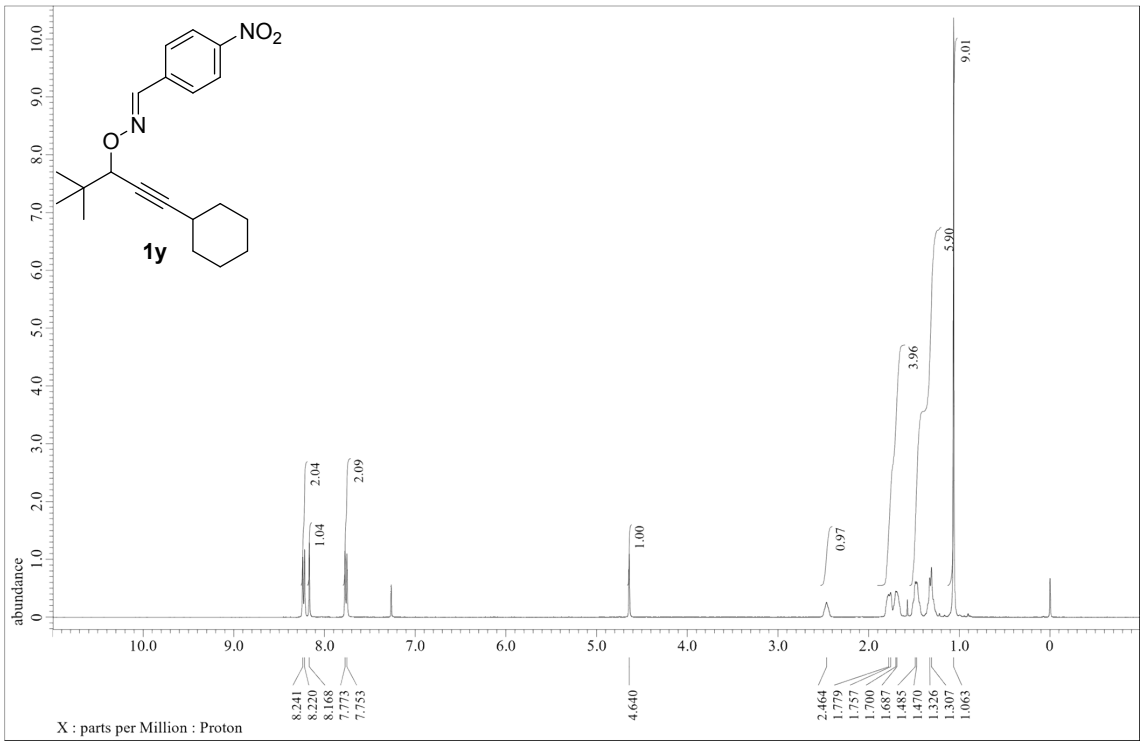

abundance
0.5
0.4
0.3
0.2
0.1
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
148.242
146.717
138.298
131.757
128.363
128.163
127.638
123.872
122.566
86.964
86.544
79.832
41.836
28.927
28.088
26.276
25.847
25.752
X : parts per Million : Carbon13

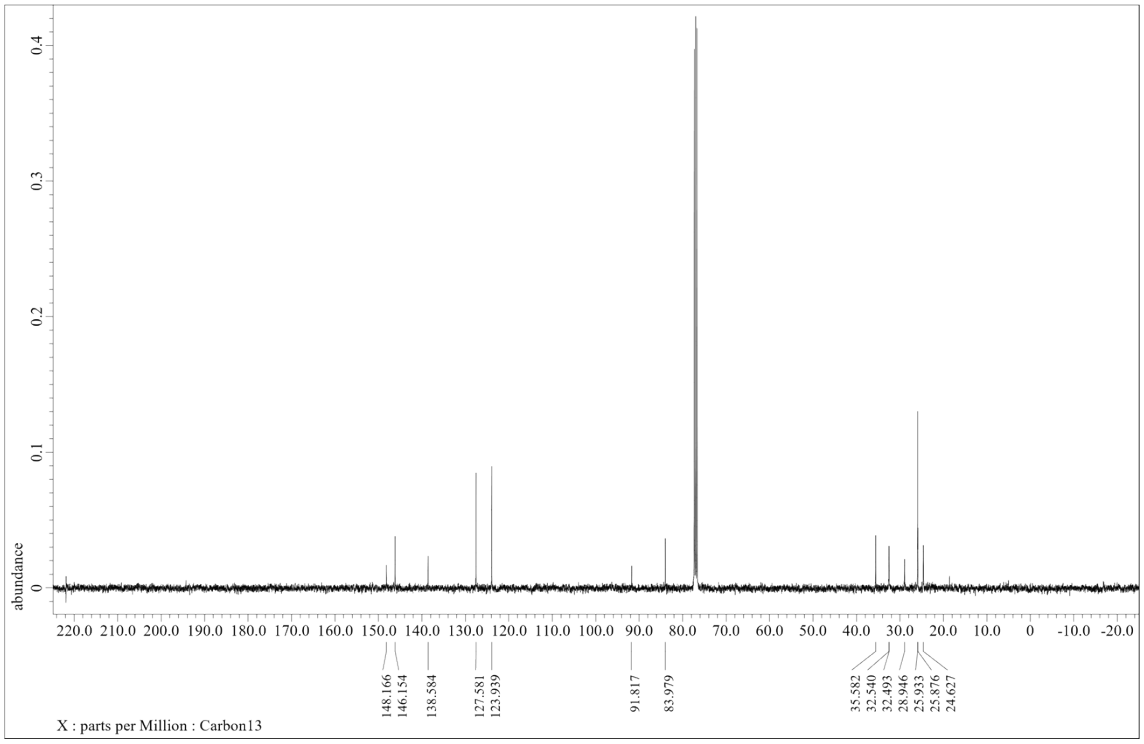

NO2
N
O
Ph
1w
abundance
4.0
3.0
2.0
1.0
0
3.04
2.04
2.02
3.06
1.00
1.01
4.04
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.243
8.220
8.214
7.790
7.769
7.463
7.458
7.446
7.438
7.314
7.311
7.300
7.296
5.046
5.030
1.505
1.501
1.491
1.485
1.469
1.455
1.449
0.702
0.693
0.690
0.686
0.679
0.674
0.669
0.664
0.651
X : parts per Million : Proton

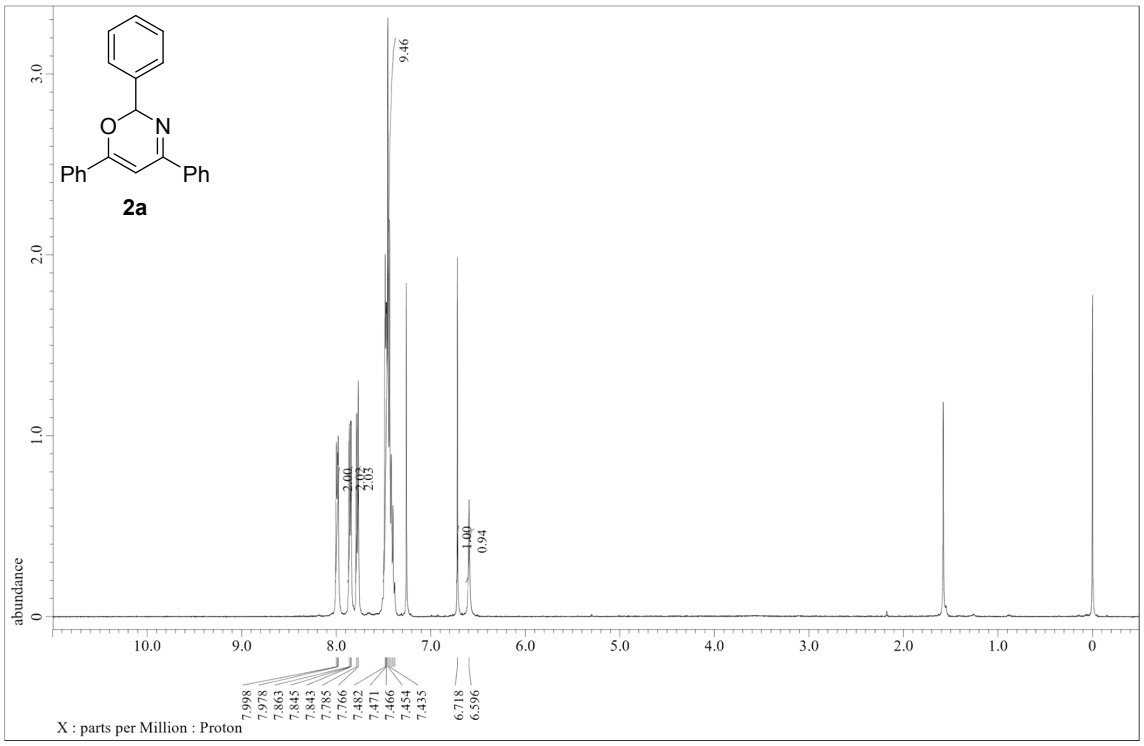

abundance
0.3
0.2
0.1
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
148.300
146.917
138.307
131.843
128.573
128.220
127.705
123.939
122.261
86.401
85.143
78.583
14.139
3.479
2.134
X : parts per Million : Carbon13

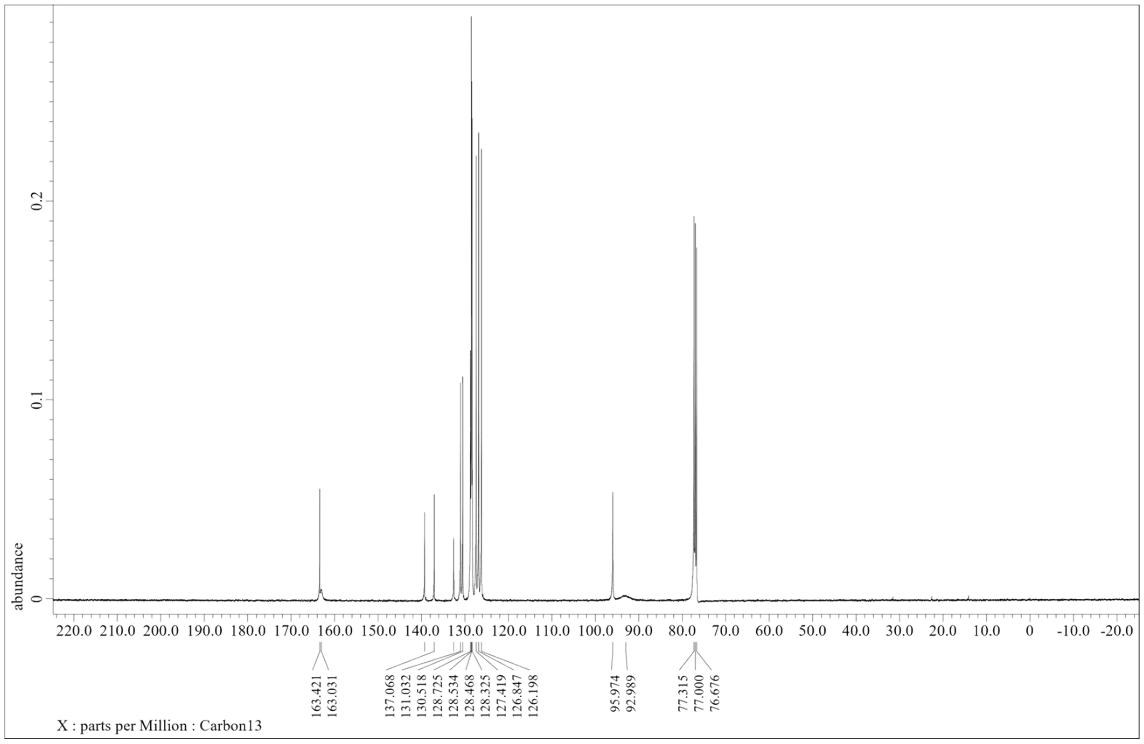

NO2
N
O
Ph
1x
abundance
X : parts per Million : Proton

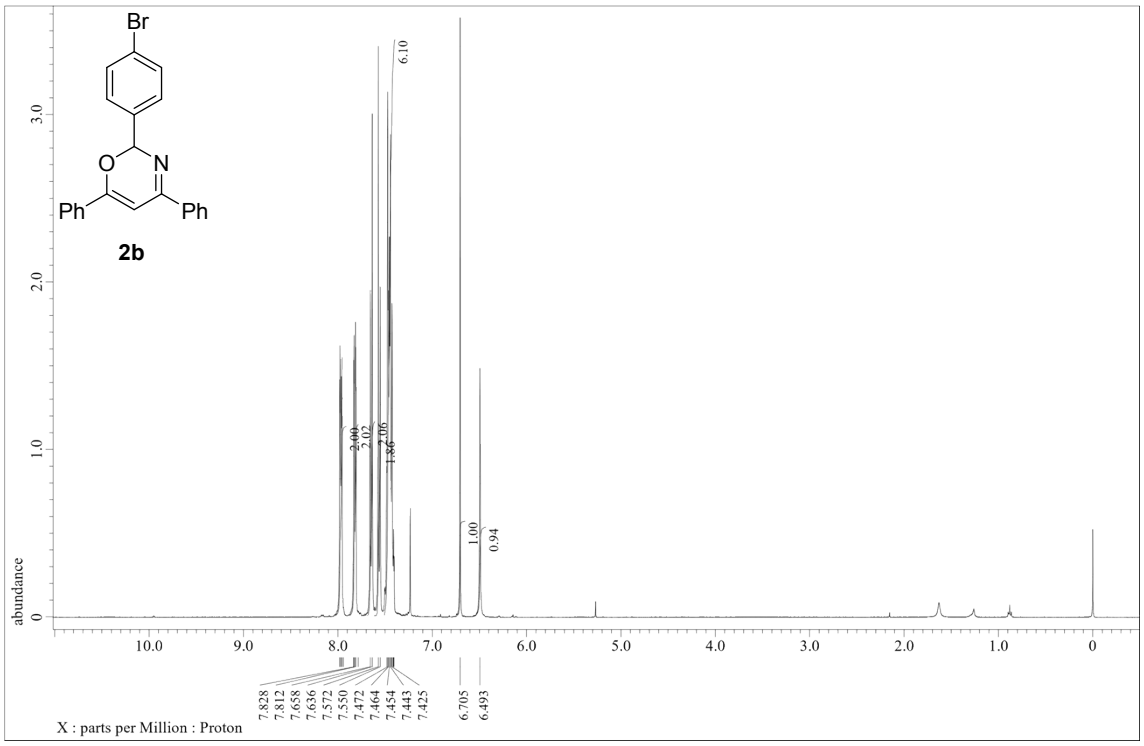

abundance
X : parts per Million : Carbon13

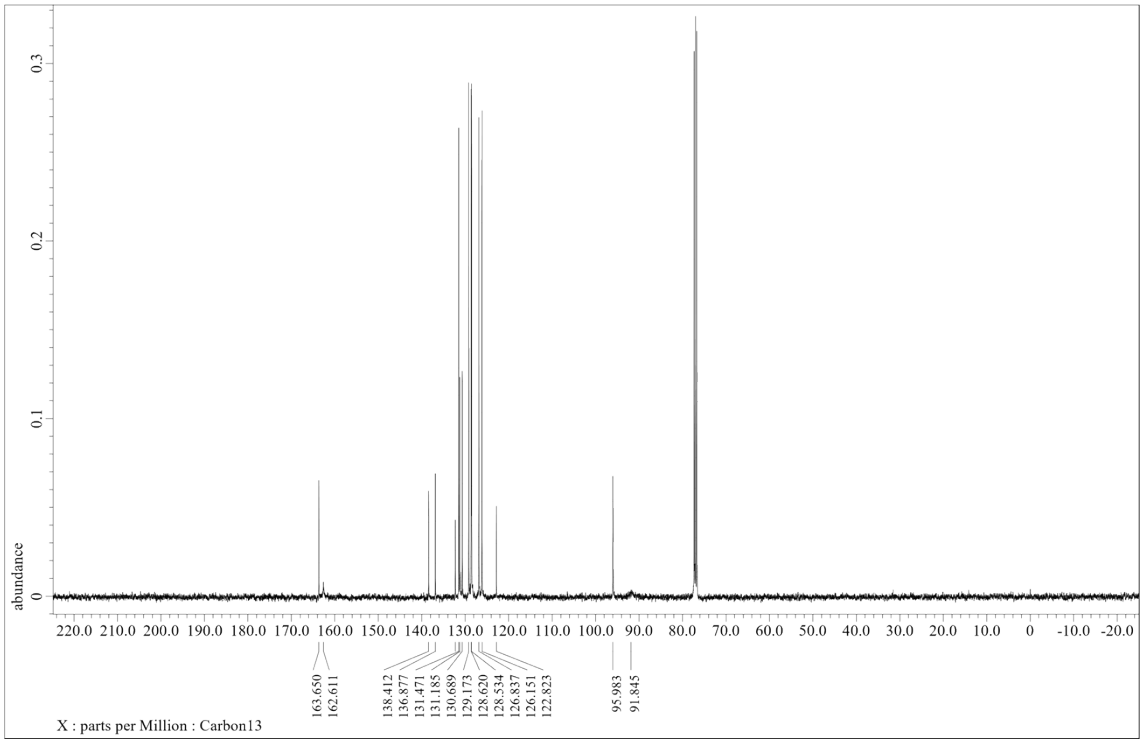

NO2
N
O
1y
abundance
9.01
5.90
3.96
2.09
2.04
1.04
1.00
0.97
8.241
8.220
8.168
7.773
7.753
4.640
2.464
1.779
1.757
1.700
1.687
1.485
1.470
1.326
1.307
1.063
X : parts per Million : Proton

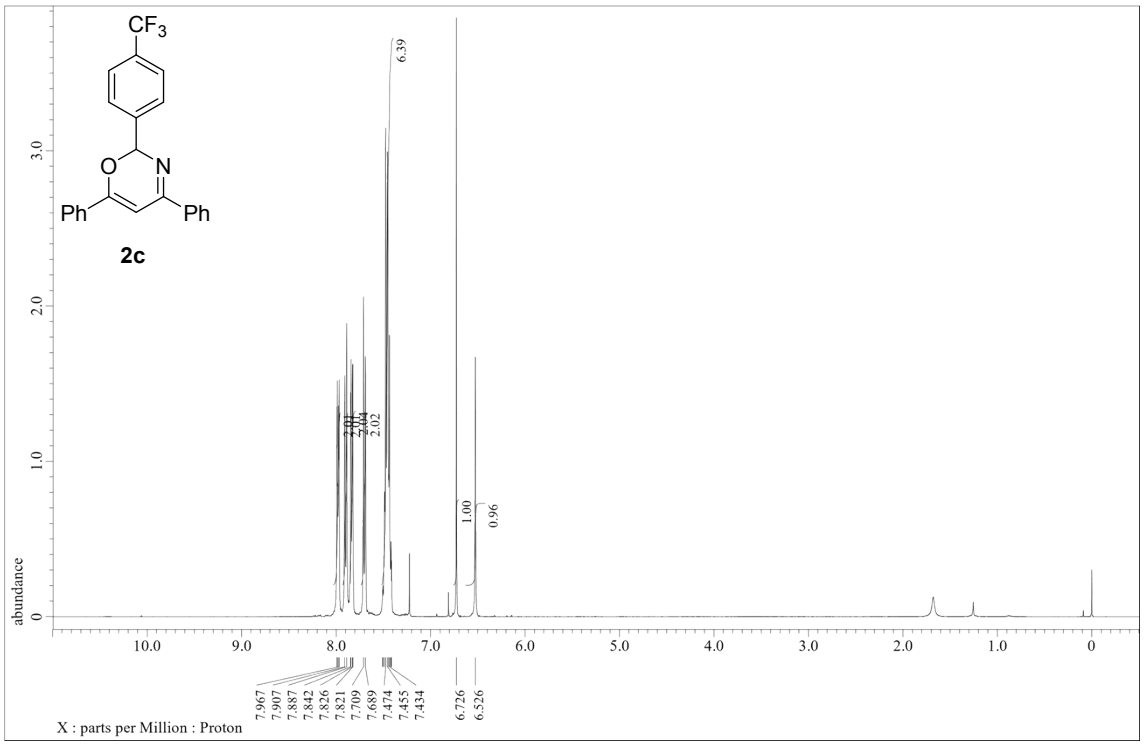

abundance
148.166
146.154
138.584
127.581
123.939
91.817
83.979
35.582
32.540
32.493
28.946
25.933
25.876
24.627
X : parts per Million : Carbon13

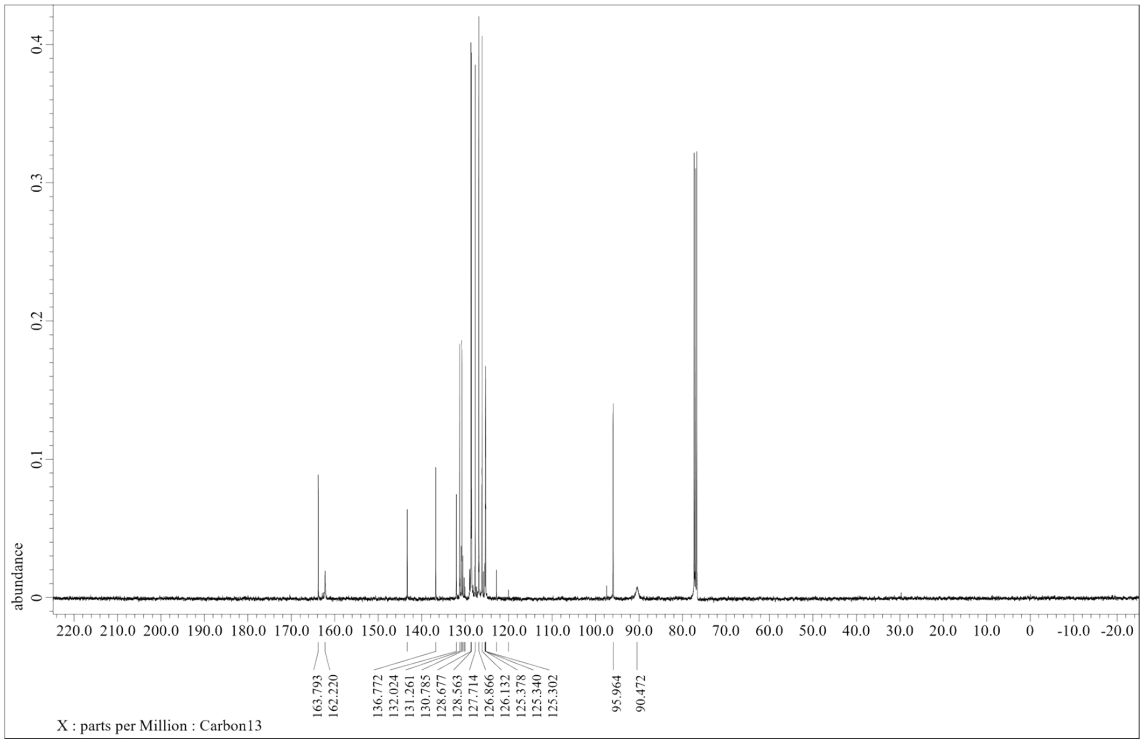

O
N
Ph
Ph
2a
9.46
2.00
2.02
2.03
1.00
0.94
abundance
7.998
7.978
7.863
7.845
7.843
7.785
7.766
7.482
7.471
7.466
7.454
7.435
6.718
6.596
X : parts per Million : Proton

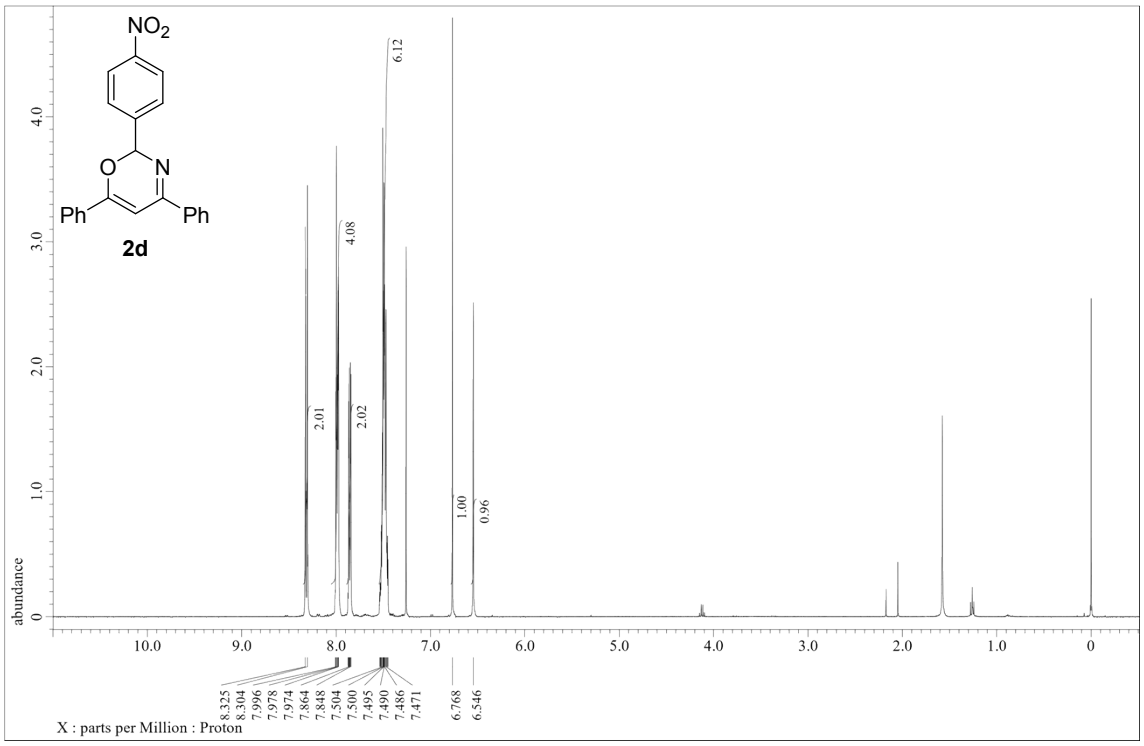

abundance
163.421
163.031
137.068
131.032
130.518
128.725
128.534
128.468
128.325
127.419
126.847
126.198
95.974
92.989
77.315
77.000
76.676
X : parts per Million : Carbon13

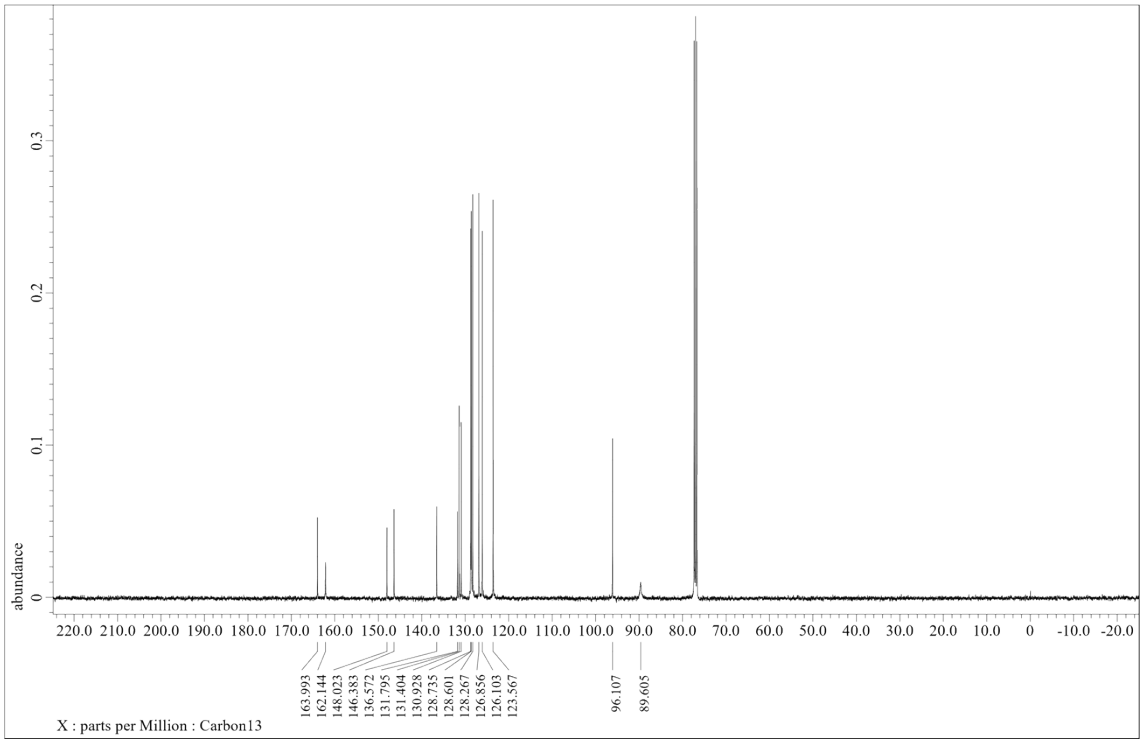

Br
O
N
Ph
Ph
2b
6.10
2.00
2.02
1.86
1.00
0.94
abundance
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.828
7.812
7.658
7.636
7.572
7.550
7.472
7.464
7.454
7.443
7.425
6.705
6.493
X : parts per Million : Proton

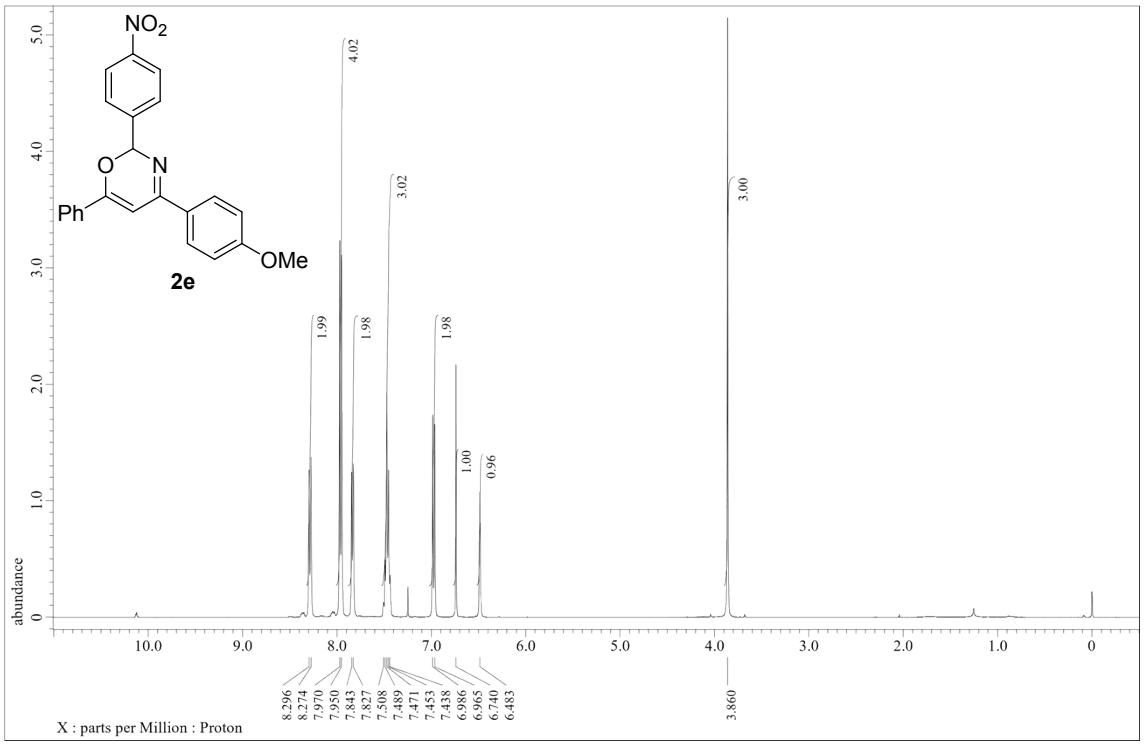

abundance
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
163.650
162.611
138.412
136.877
131.471
131.185
130.689
129.173
128.620
128.534
126.837
126.151
122.823
95.983
91.845
X : parts per Million : Carbon13

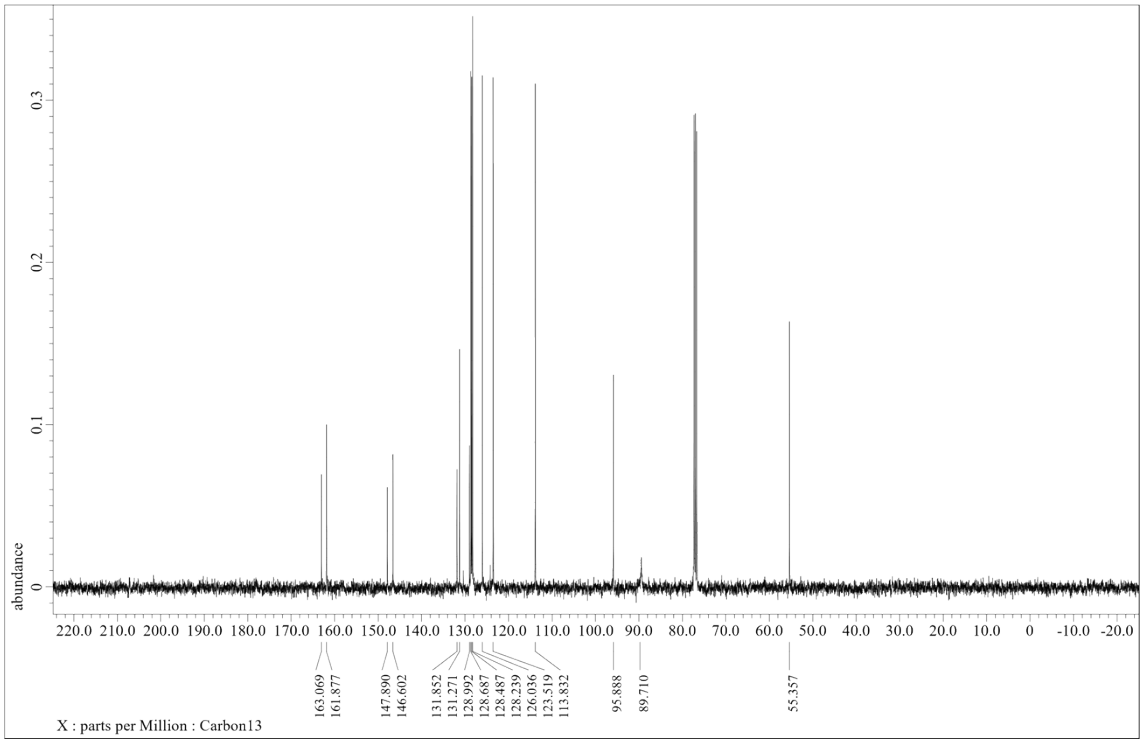

CF3
O
N
Ph
Ph
2c
6.39
2.01
2.04
2.04
2.02
1.00
0.96
abundance
3.0
2.0
1.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.967
7.907
7.887
7.842
7.826
7.821
7.709
7.689
7.474
7.455
7.434
6.726
6.526
X : parts per Million : Proton

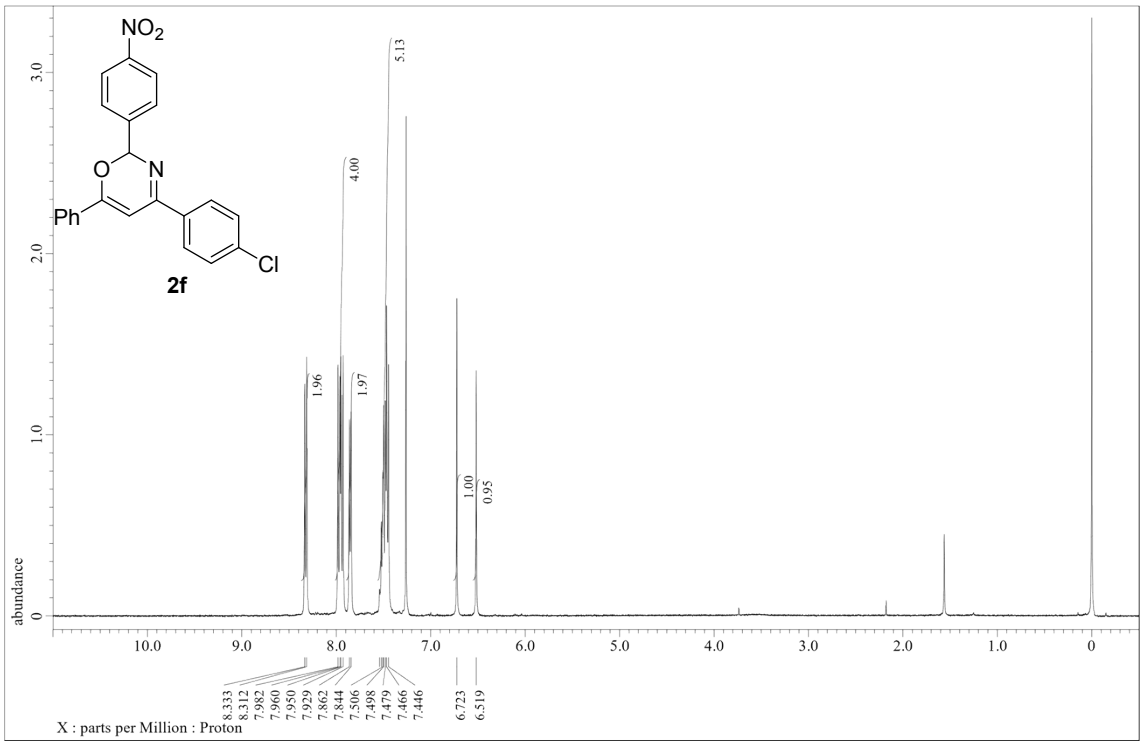

abundance
0.4
0.3
0.2
0.1
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
163.793
162.220
136.772
132.024
131.261
130.785
128.677
128.563
127.714
126.866
126.132
125.378
125.340
125.302
95.964
90.472
X : parts per Million : Carbon13

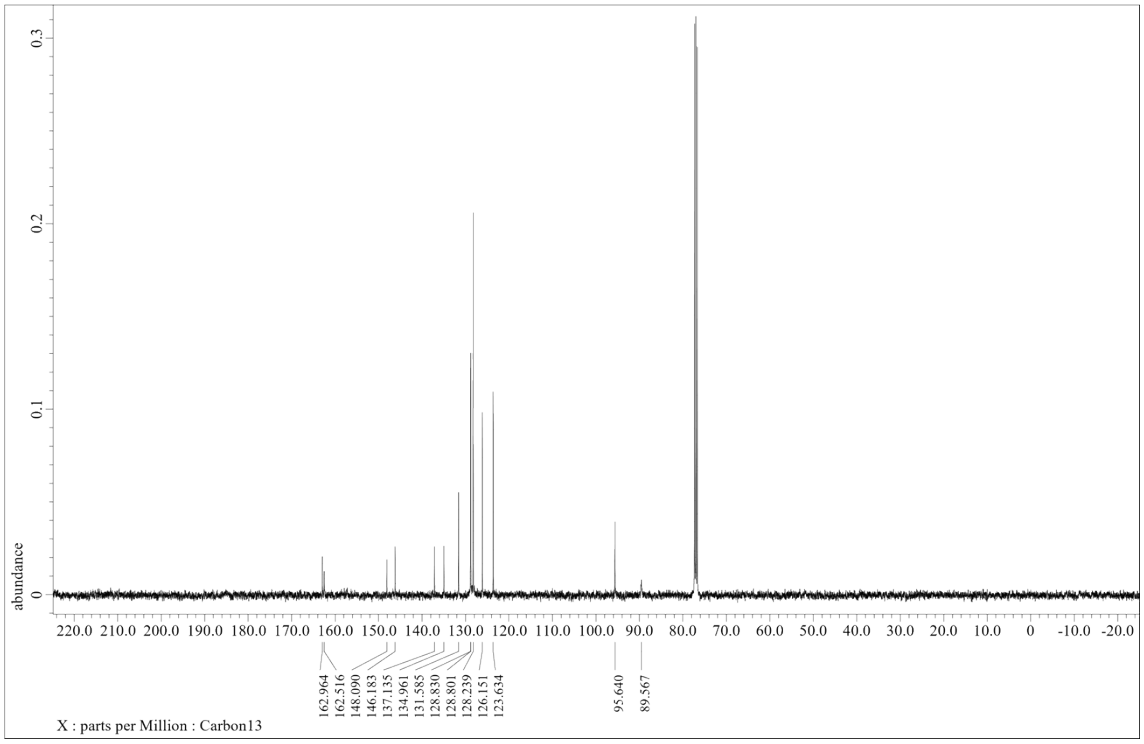

NO2
O
N
Ph
Ph
2d
6.12
4.08
2.01
2.02
1.00
0.96
abundance
8.325
8.304
7.996
7.978
7.974
7.864
7.848
7.504
7.500
7.495
7.490
7.486
7.471
6.768
6.546
X : parts per Million : Proton

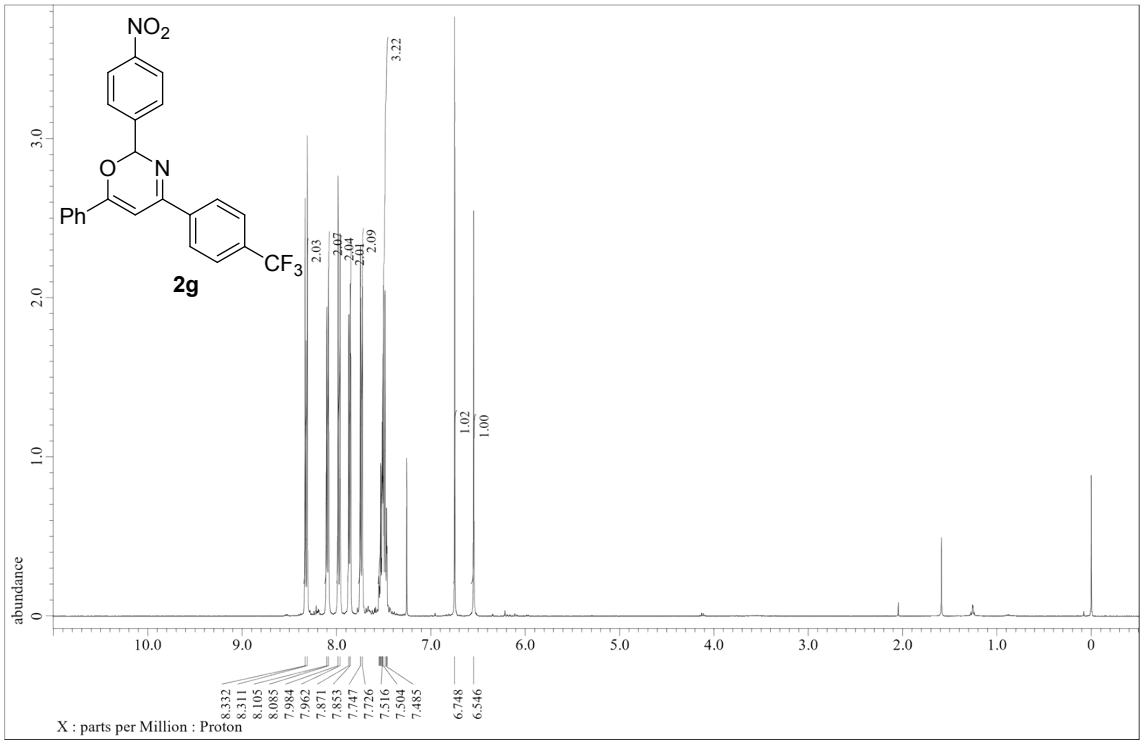

abundance
163.993
162.144
148.023
146.383
136.572
131.795
131.404
130.928
128.735
128.601
128.267
126.856
126.103
123.567
96.107
89.605
X : parts per Million : Carbon13

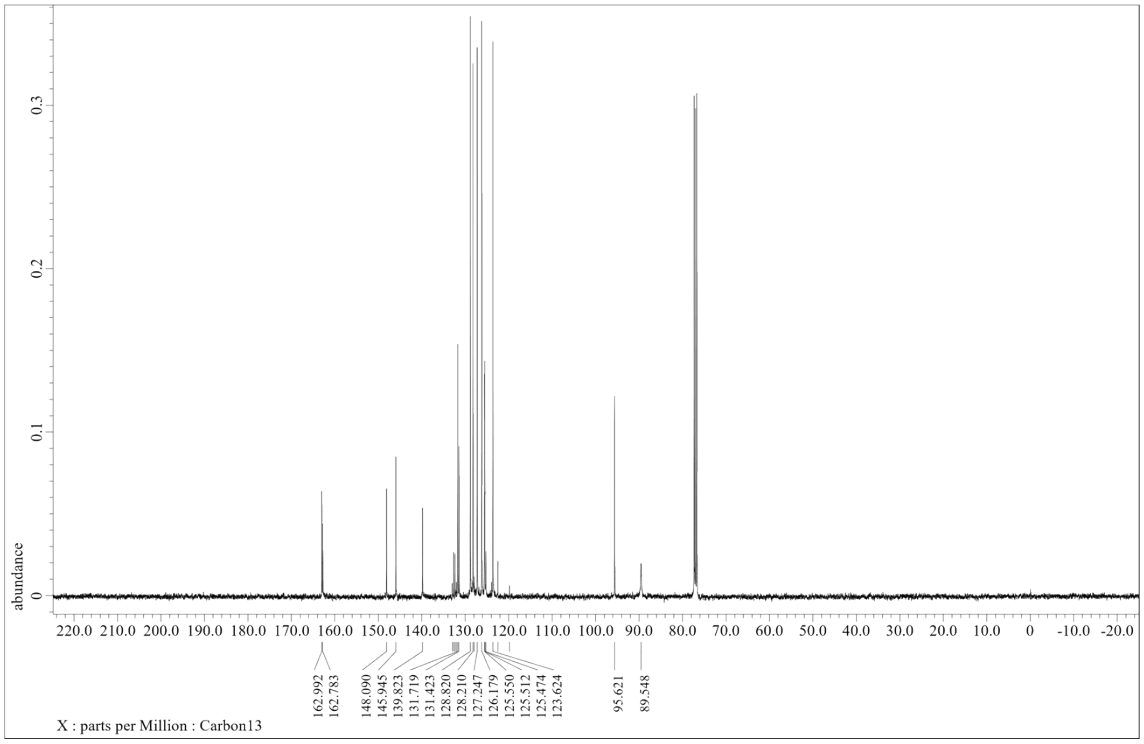

NO2
O
N
Ph
OMe
2e
4.02
3.02
3.00
1.99
1.98
1.98
1.00
0.96
abundance
8.296
8.274
7.970
7.950
7.843
7.827
7.508
7.489
7.471
7.453
7.438
6.986
6.965
6.740
6.483
3.860
X : parts per Million : Proton

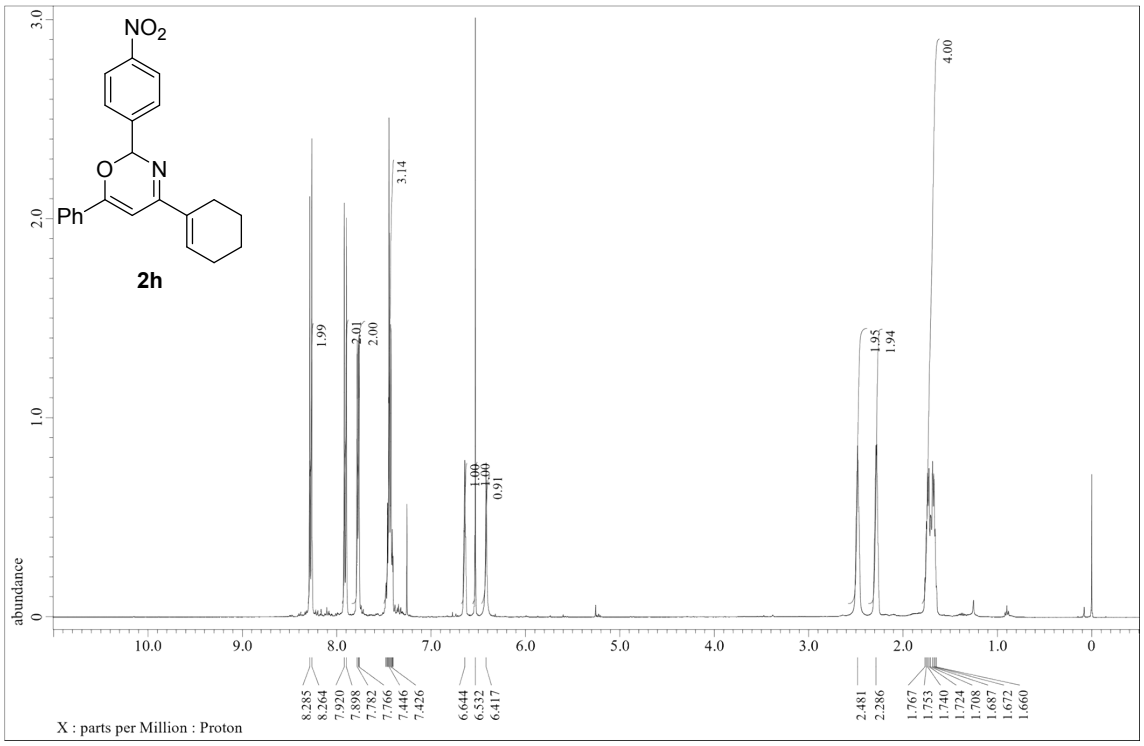

abundance
163.069
161.877
147.890
146.602
131.852
131.271
128.992
128.687
128.487
128.239
126.036
123.519
113.832
95.888
89.710
55.357
X : parts per Million : Carbon13

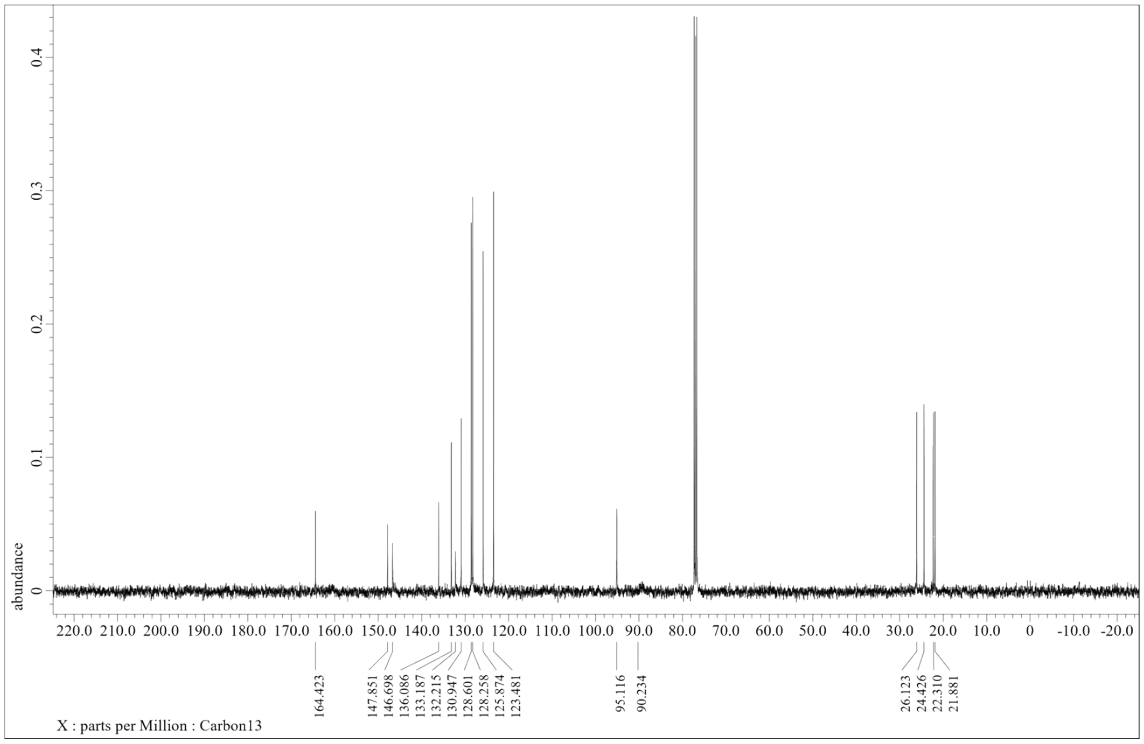

NO2
O
N
Ph
Cl
2f
abundance
X : parts per Million : Proton

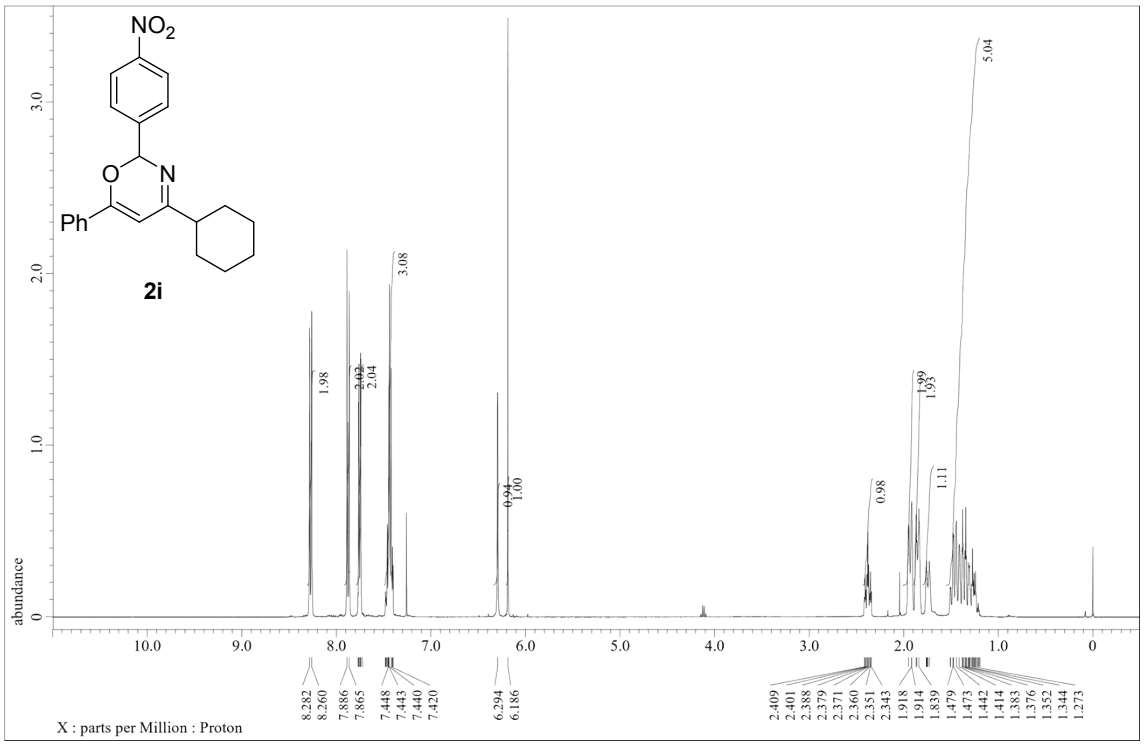

abundance
X : parts per Million : Carbon13

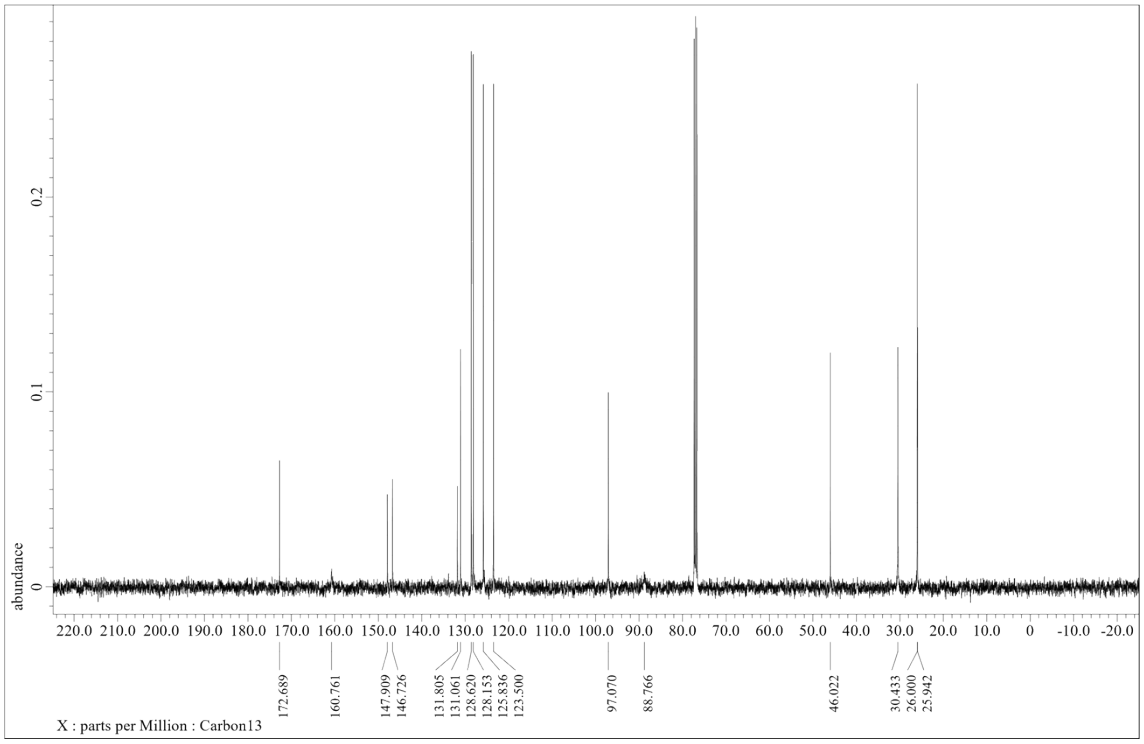

NO2
O
N
Ph
CF3
2g
3.22
2.03
2.07
2.04
2.01
2.09
1.02
1.00
abundance
8.332
8.311
8.105
8.085
7.984
7.962
7.871
7.853
7.747
7.726
7.516
7.504
7.485
6.748
6.546
X : parts per Million : Proton

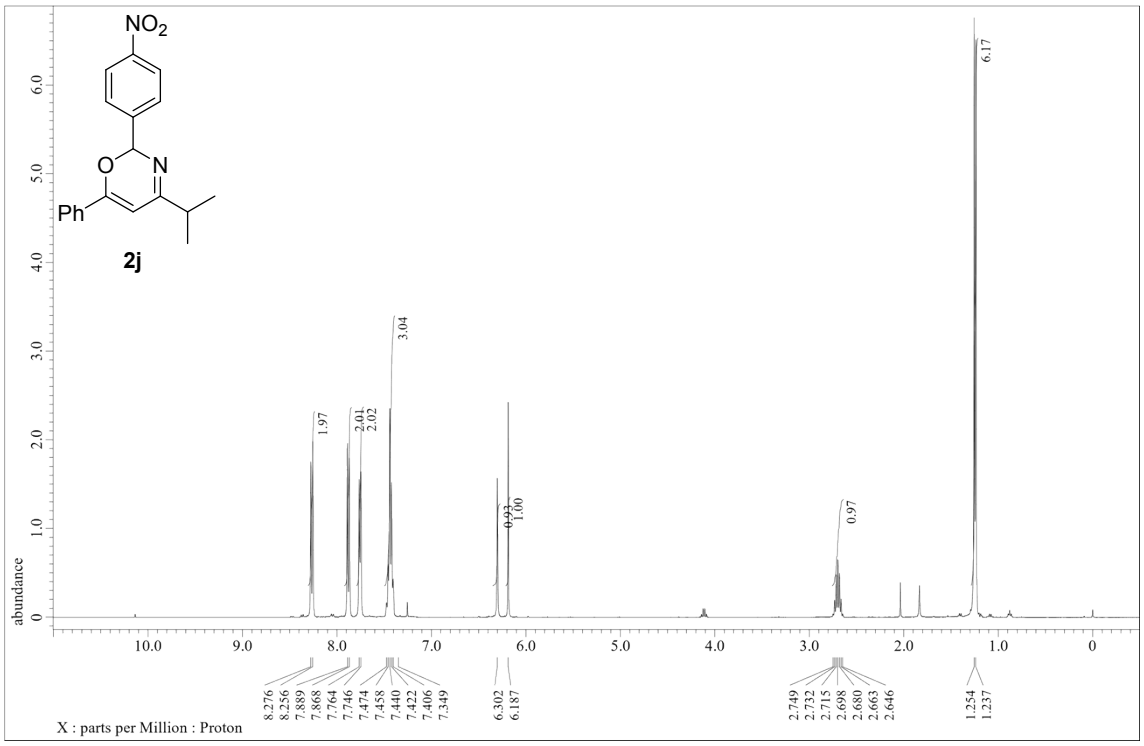

abundance
162.992
162.783
148.090
145.945
139.823
131.719
131.423
128.820
128.210
127.247
126.179
125.550
125.512
125.474
123.624
95.621
89.548
X : parts per Million : Carbon13

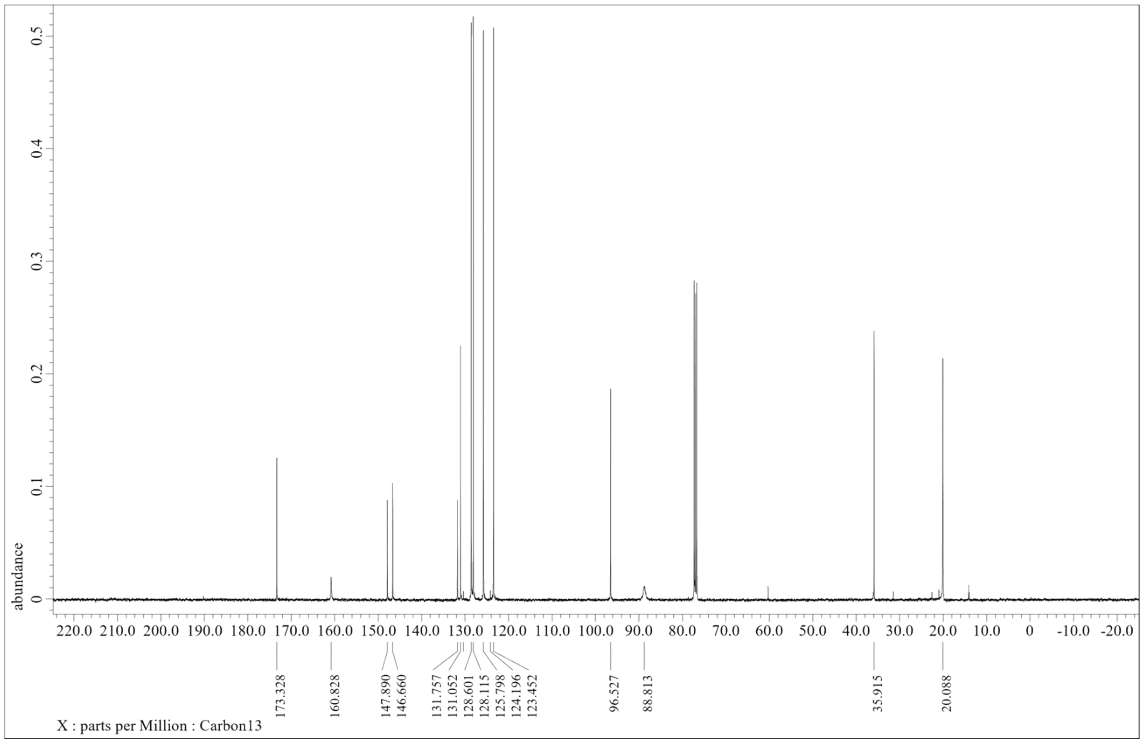

NO2
O
N
Ph
2h
abundance
X : parts per Million : Proton

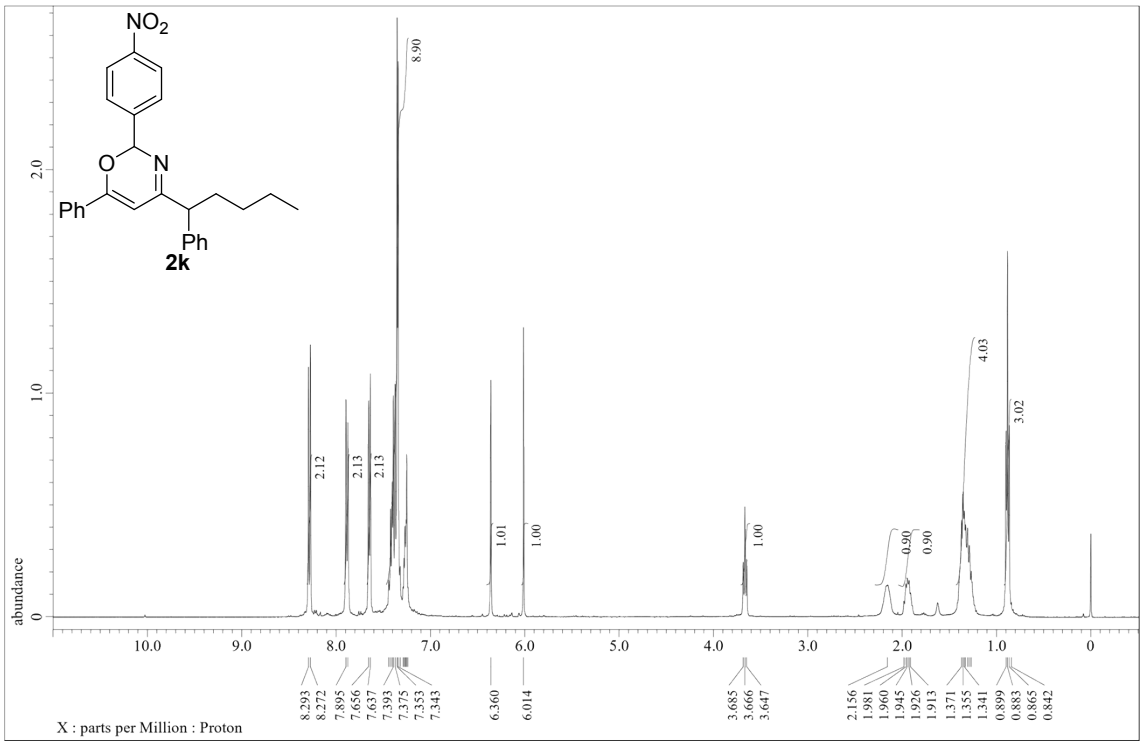

abundance
X : parts per Million : Carbon13

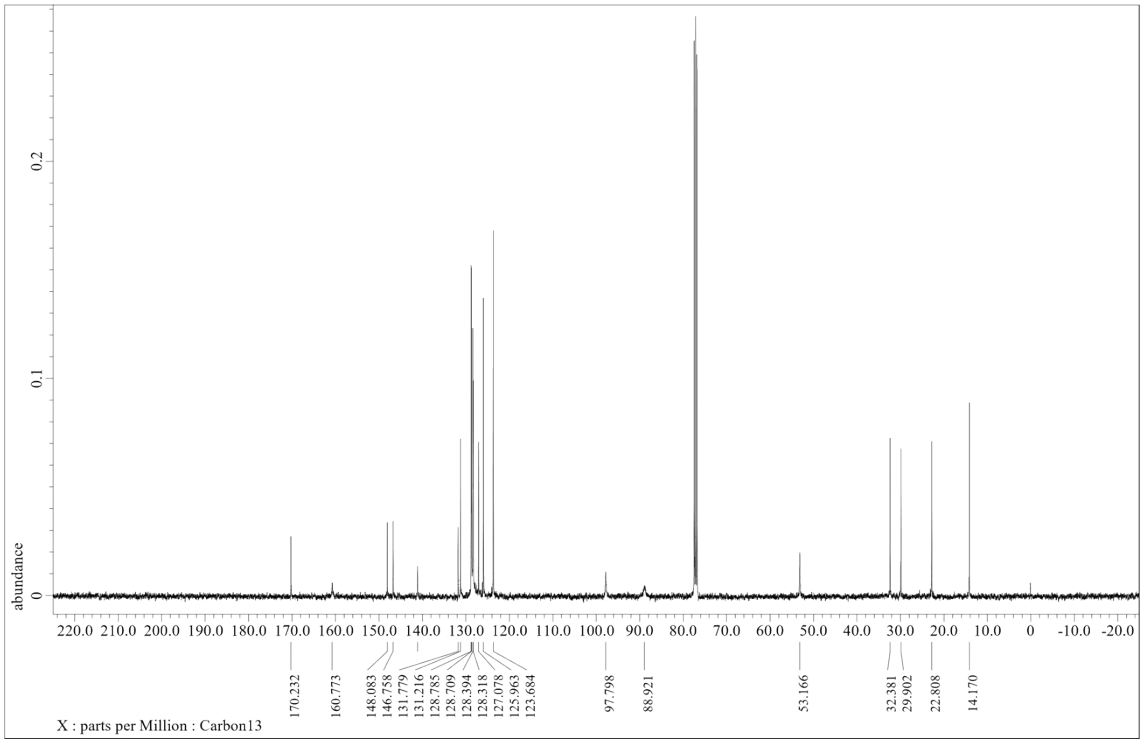

NO2
O
N
Ph
2i
abundance
X : parts per Million : Proton

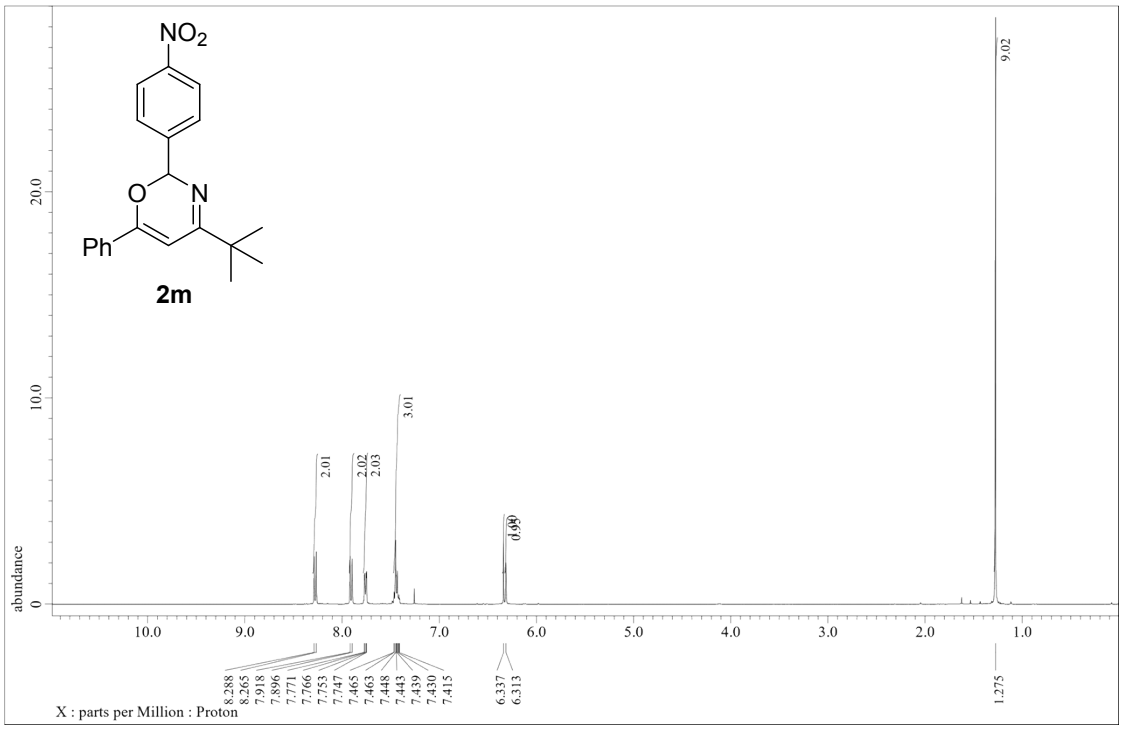

abundance
X : parts per Million : Carbon13

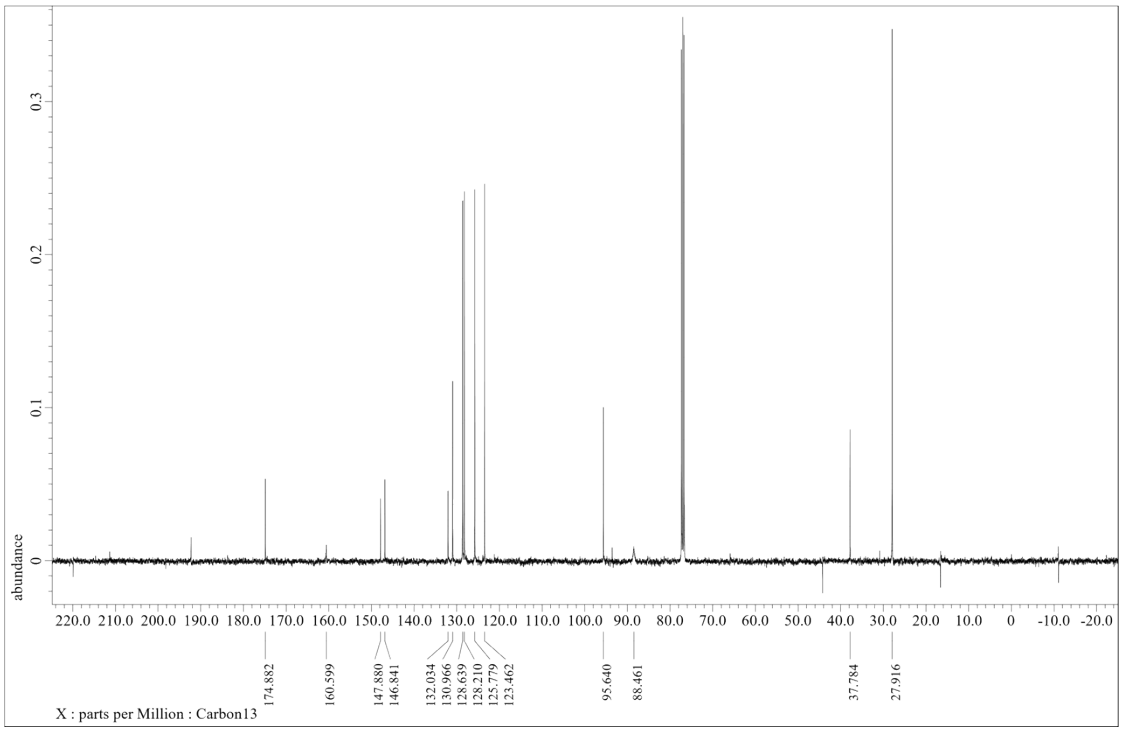

NO2
O
N
Ph
2j
abundance
X : parts per Million : Proton
8.276
8.256
7.889
7.868
7.764
7.746
7.474
7.458
7.440
7.422
7.406
7.349
6.302
6.187
2.749
2.732
2.715
2.698
2.680
2.663
2.646
1.254
1.237

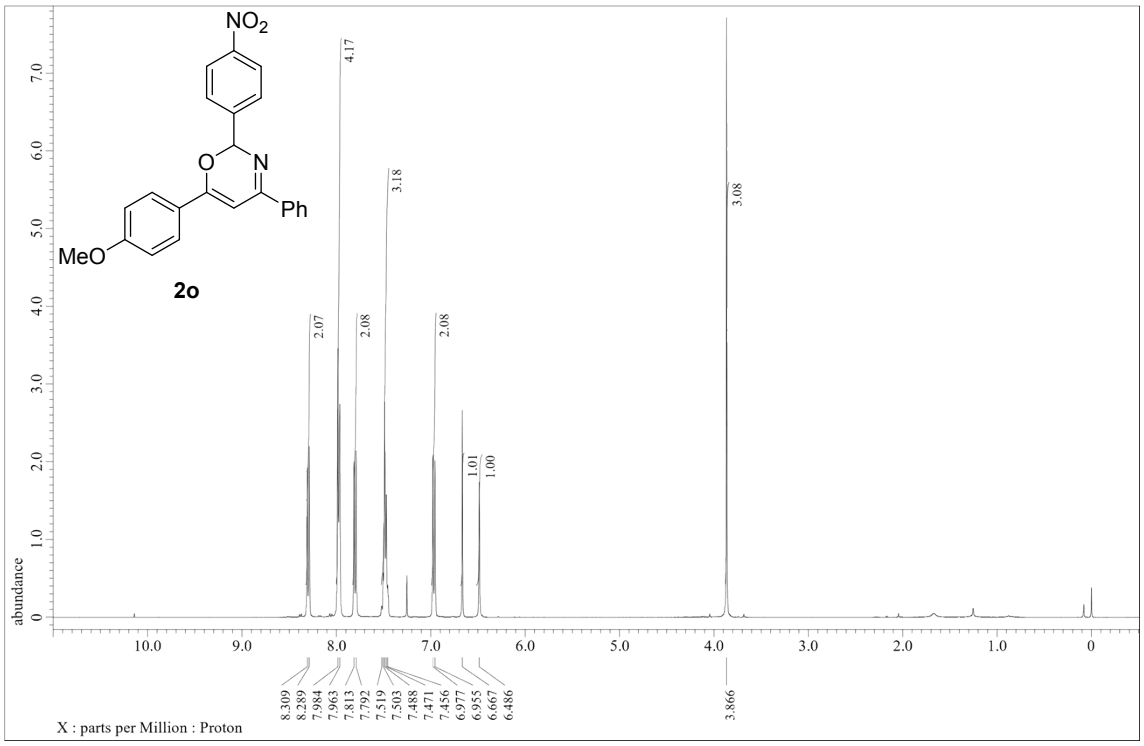

abundance
X : parts per Million : Carbon13
173.328
160.828
147.890
146.660
131.757
131.052
128.601
128.115
125.798
124.196
123.452
96.527
88.813
35.915
20.088

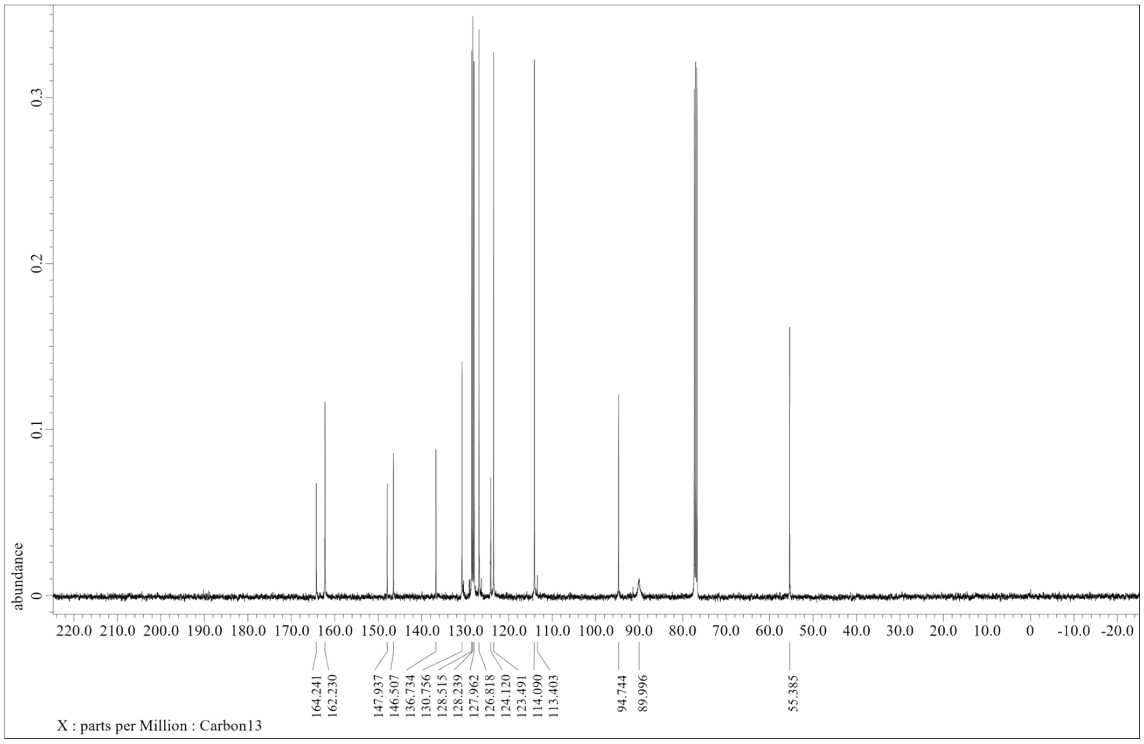

NO2
O
N
Ph
Ph
2k
abundance
X : parts per Million : Proton

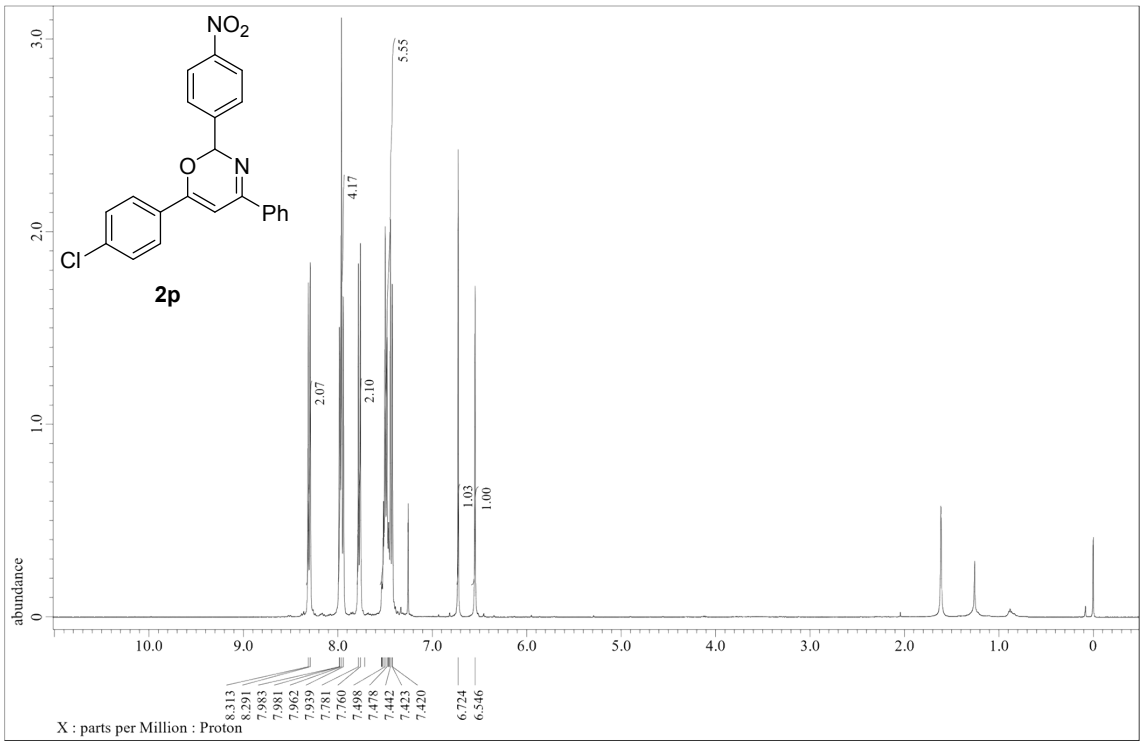

abundance
X : parts per Million : Carbon13

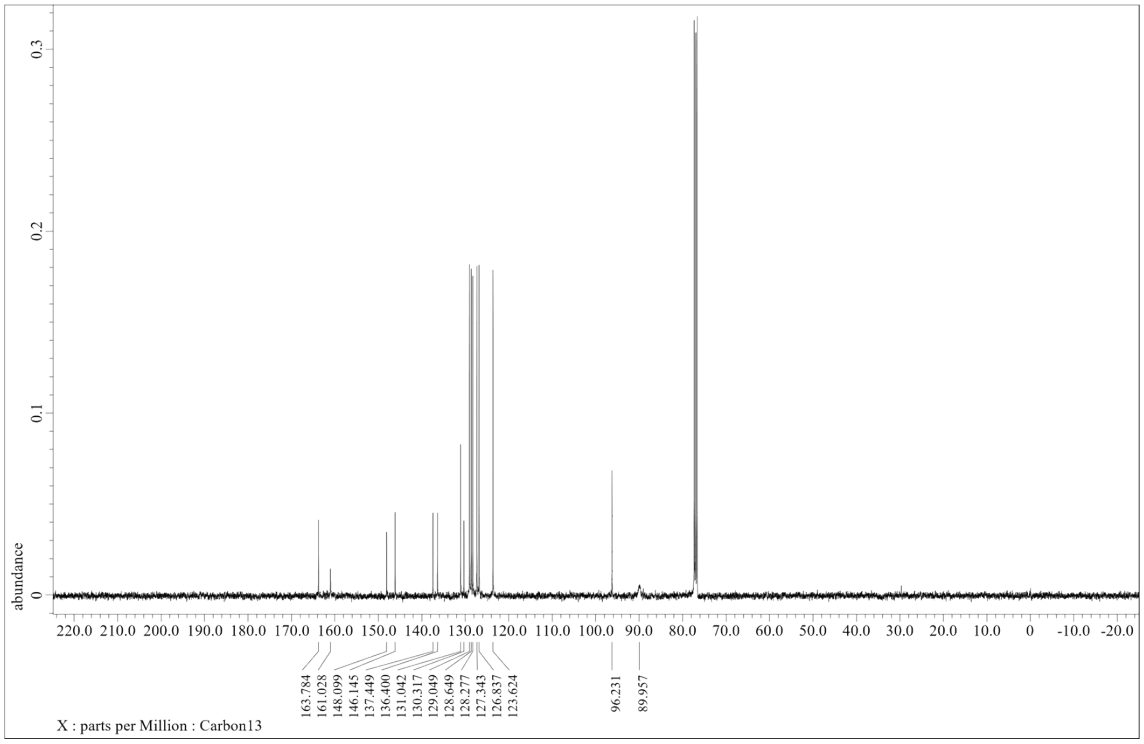

NO2
O
N
Ph
2m
abundance
20.0
10.0
0
2.01
2.02
2.03
3.01
1.00
0.99
9.02
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
8.288
8.265
7.918
7.896
7.771
7.766
7.753
7.747
7.465
7.463
7.448
7.443
7.439
7.430
7.415
6.337
6.313
1.275
X : parts per Million : Proton

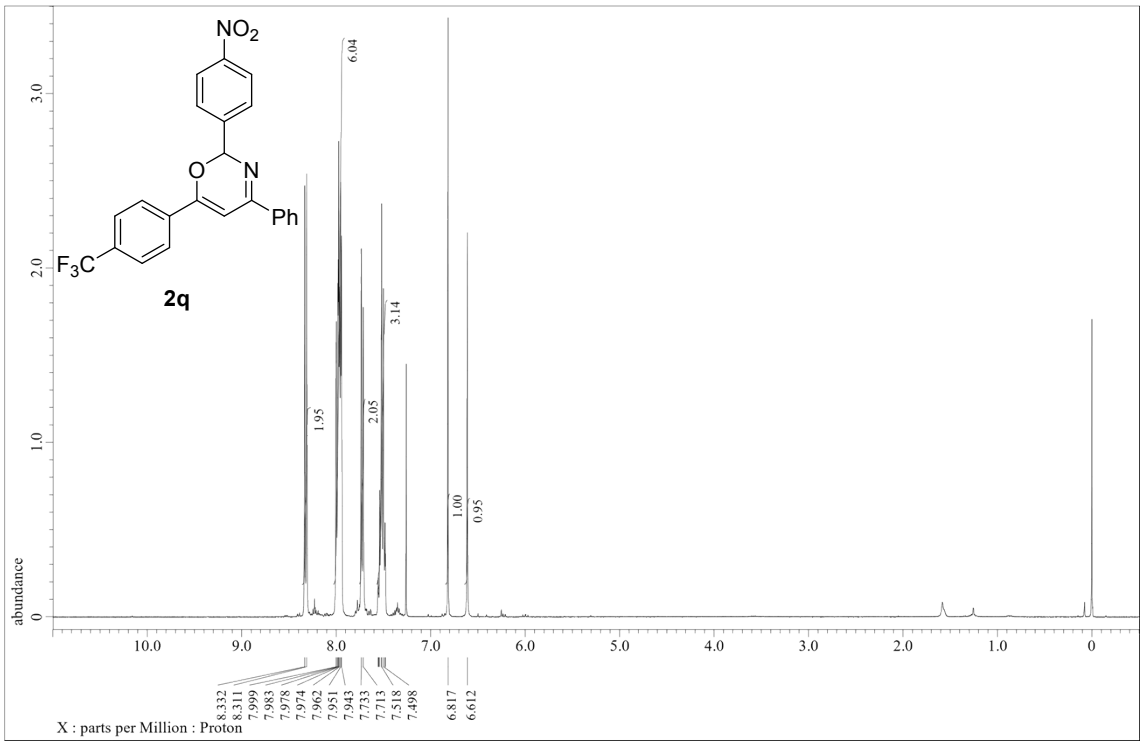

abundance
0.3
0.2
0.1
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
174.882
160.599
147.880
146.841
132.034
130.966
128.639
128.210
125.779
123.462
95.640
88.461
37.784
27.916
X : parts per Million : Carbon13

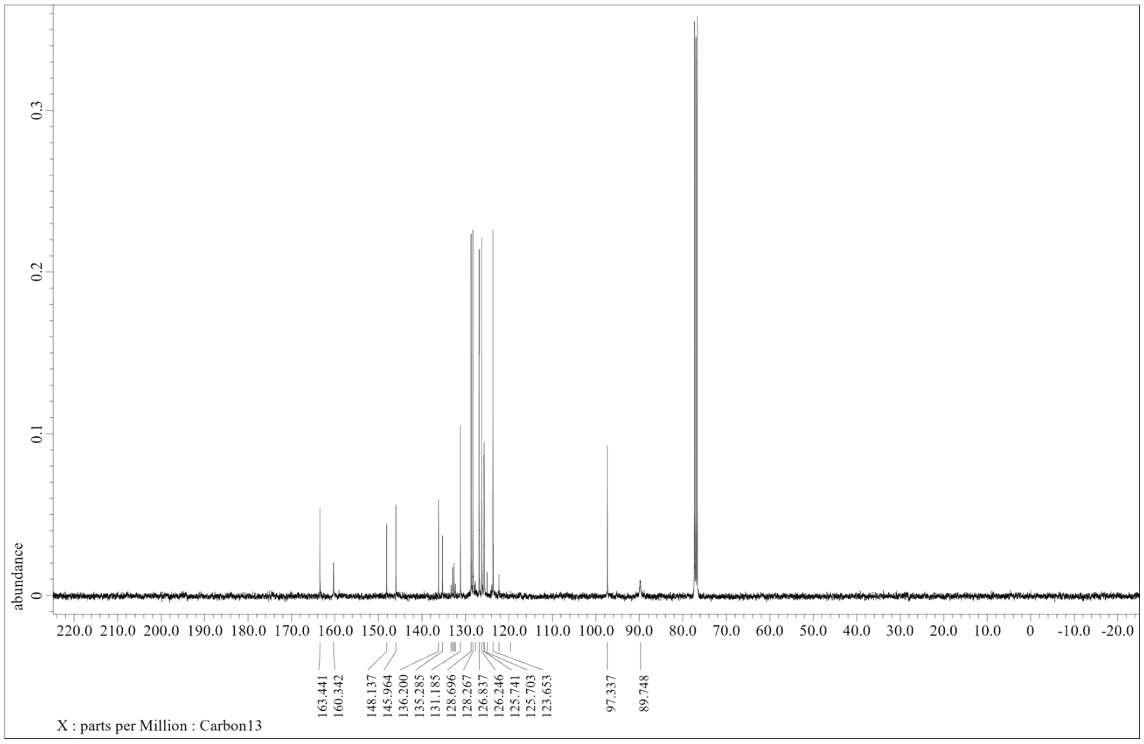

NO2
O
N
Ph
MeO
2o
4.17
3.18
3.08
2.07
2.08
2.08
1.01
1.00
abundance
8.309
8.289
7.984
7.963
7.813
7.792
7.519
7.503
7.488
7.471
7.456
6.977
6.955
6.667
6.486
3.866
X : parts per Million : Proton

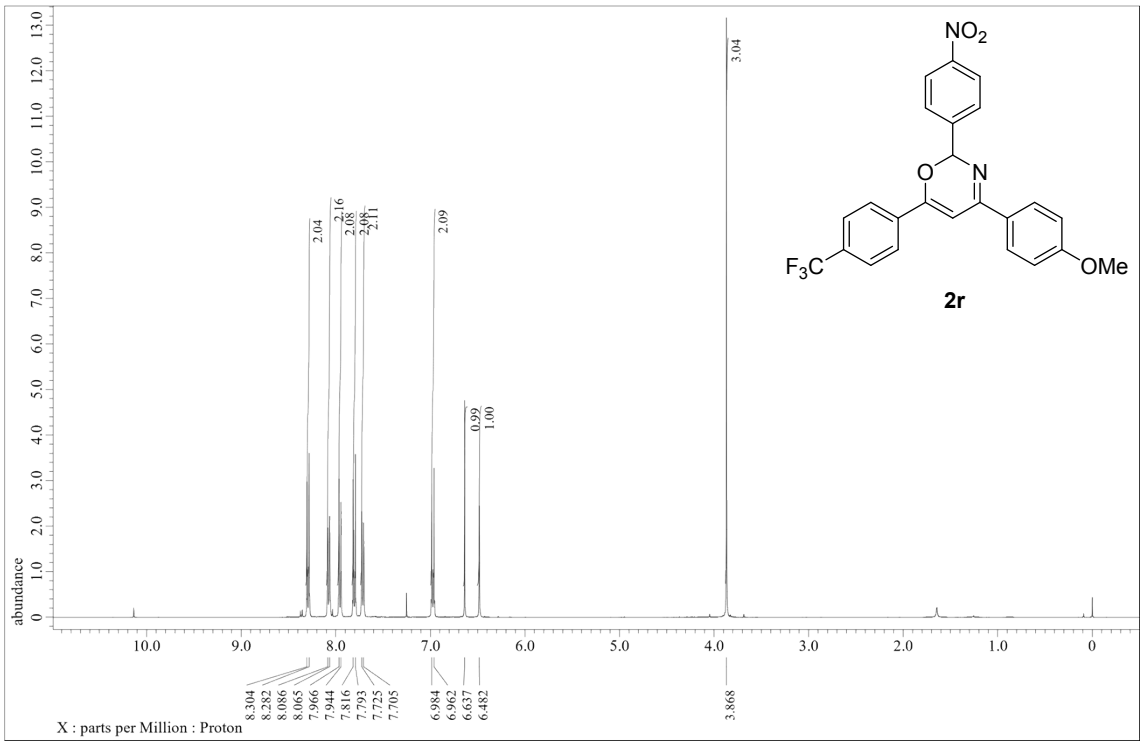

abundance
164.241
162.230
147.937
146.507
136.734
130.756
128.515
128.239
127.962
126.818
124.120
123.491
114.090
113.403
94.744
89.996
55.385
X : parts per Million : Carbon13

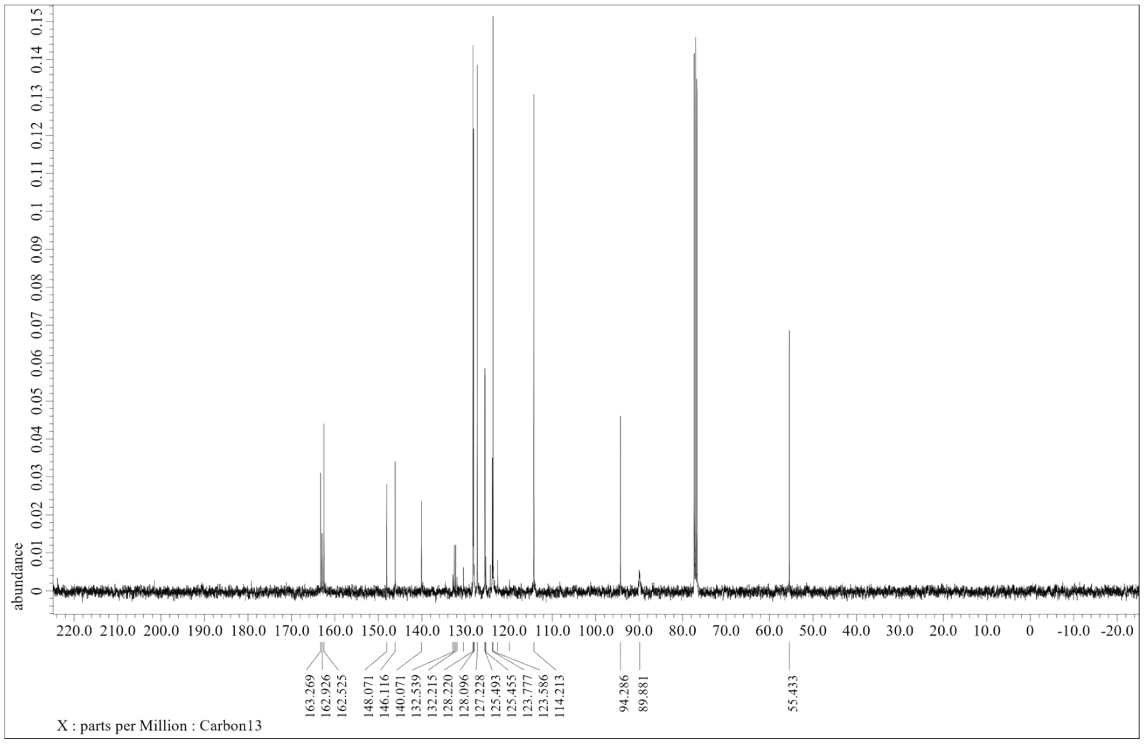

NO2
O
N
Ph
Cl
2p
abundance
X : parts per Million : Proton
2.07
4.17
2.10
5.55
1.03
1.00
8.313
8.291
7.983
7.981
7.962
7.939
7.781
7.760
7.498
7.478
7.442
7.423
7.420
6.724
6.546

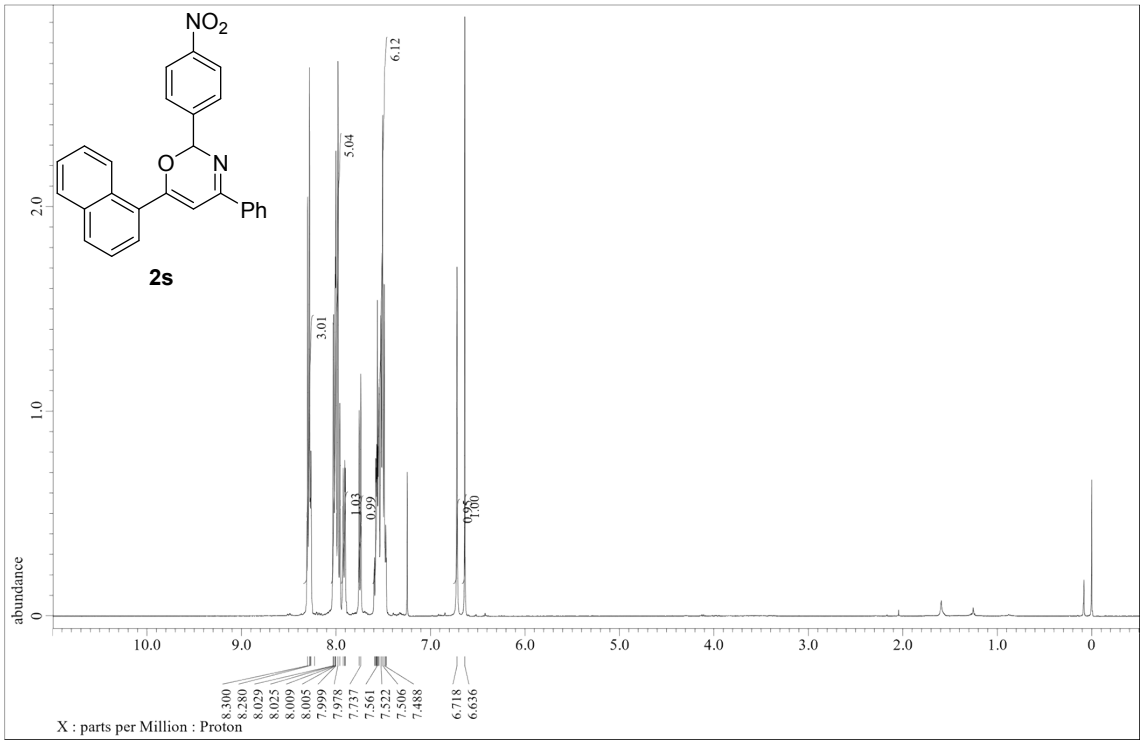

abundance
X : parts per Million : Carbon13
163.784
161.028
148.099
146.145
137.449
136.400
131.042
130.317
129.049
128.649
128.277
127.343
126.837
123.624
96.231
89.957

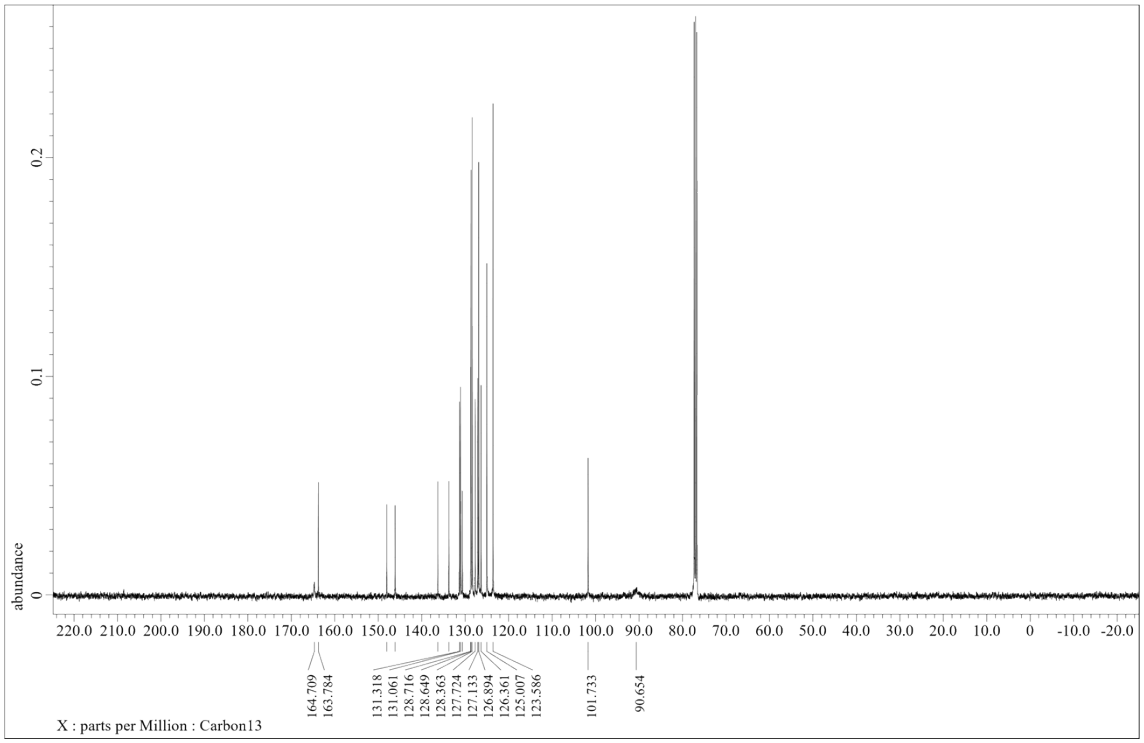

NO2
O
N
Ph
F3C
2q
6.04
3.14
1.95
2.05
1.00
0.95
abundance
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.332
8.311
7.999
7.983
7.978
7.974
7.962
7.951
7.943
7.733
7.713
7.518
7.498
6.817
6.612
X : parts per Million : Proton

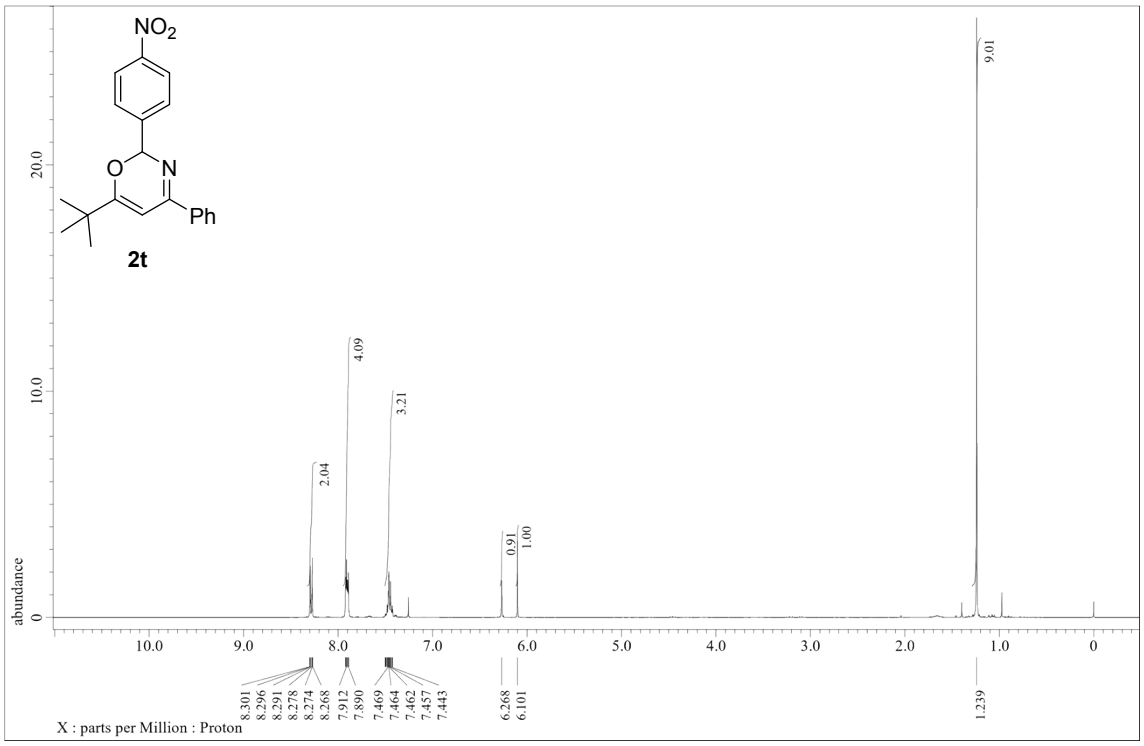

abundance
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
163.441
160.342
148.137
145.964
136.200
135.285
131.185
128.696
128.267
126.837
126.246
125.741
125.703
123.653
97.337
89.748
X : parts per Million : Carbon13

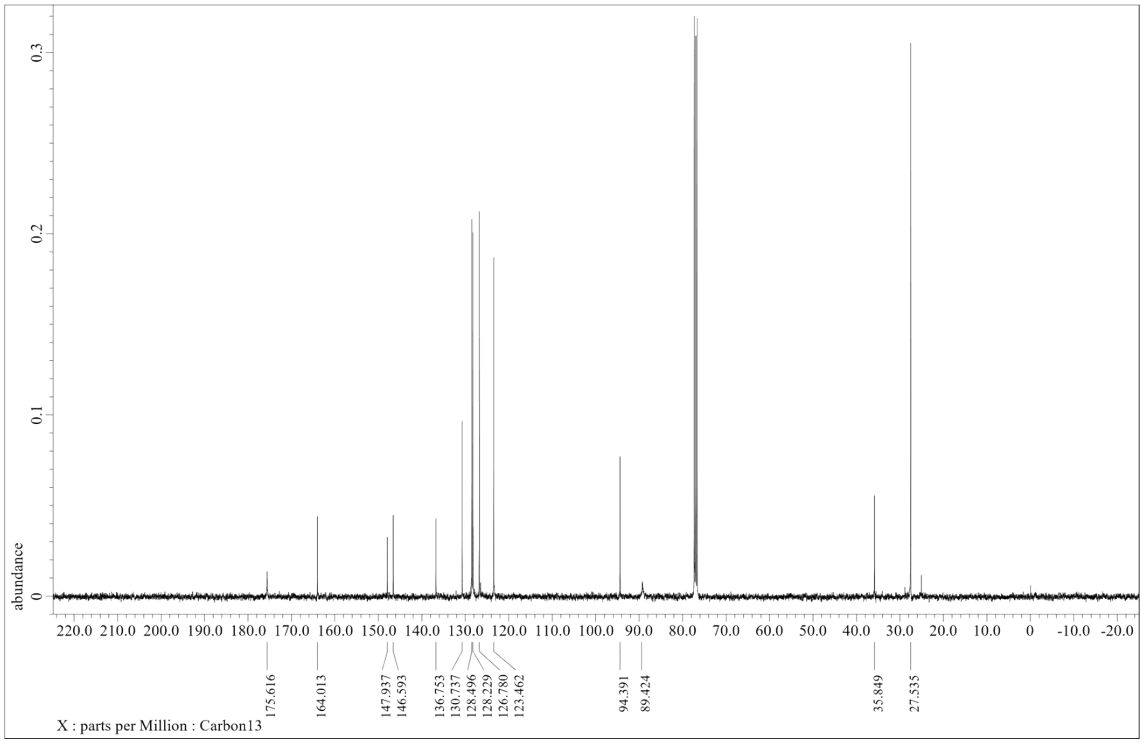

NO2
O
N
F3C
OMe
2r
abundance
X : parts per Million : Proton

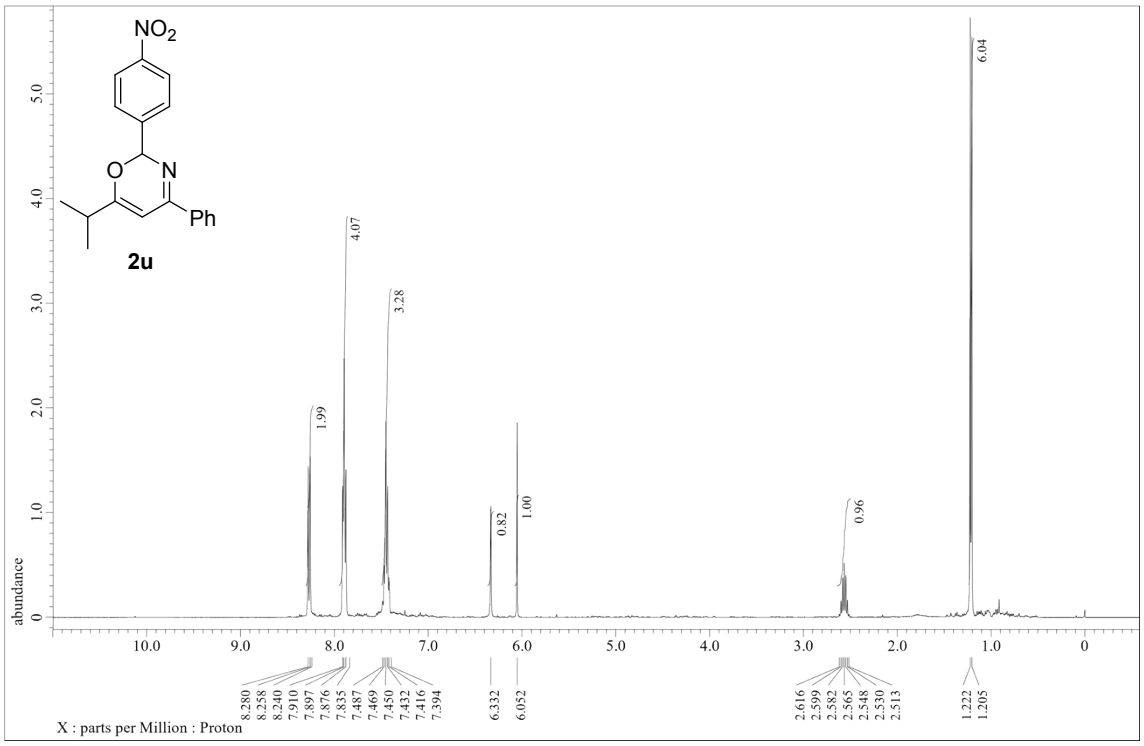

abundance
X : parts per Million : Carbon13

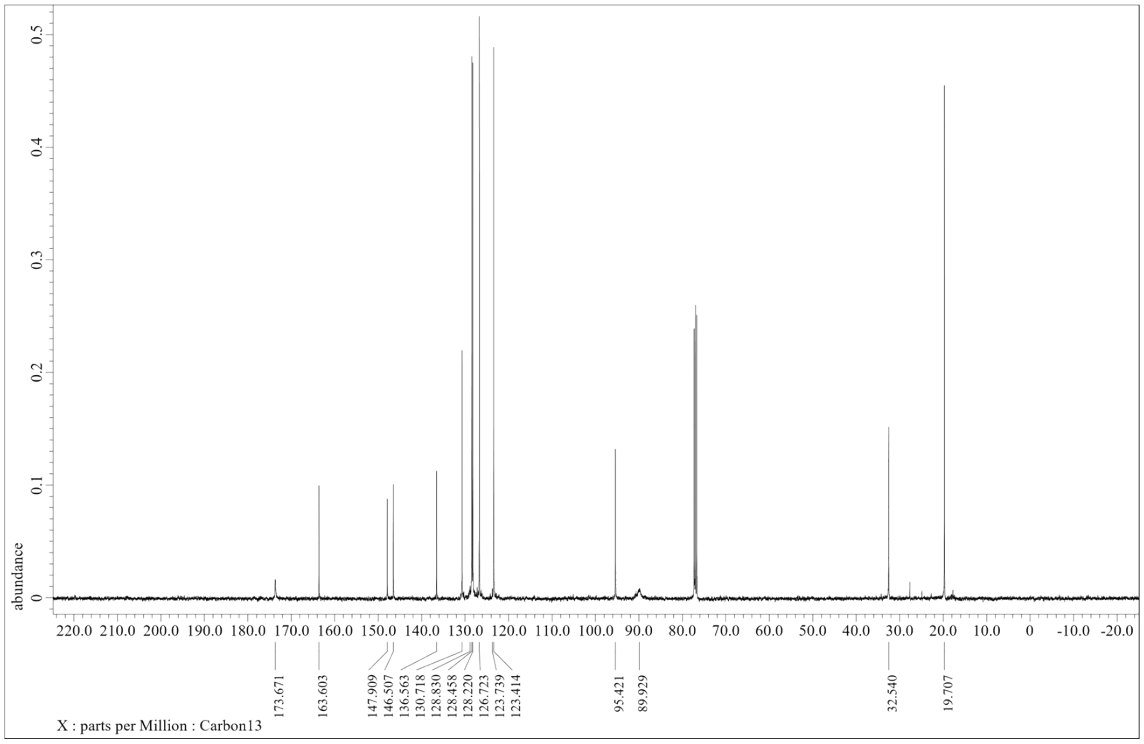

NO2
O
N
Ph
2s
6.12
5.04
3.01
1.03
0.99
0.96
1.00
abundance
2.0
1.0
0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.300
8.280
8.029
8.025
8.009
8.005
7.999
7.978
7.737
7.561
7.522
7.506
7.488
6.718
6.636
X : parts per Million : Proton

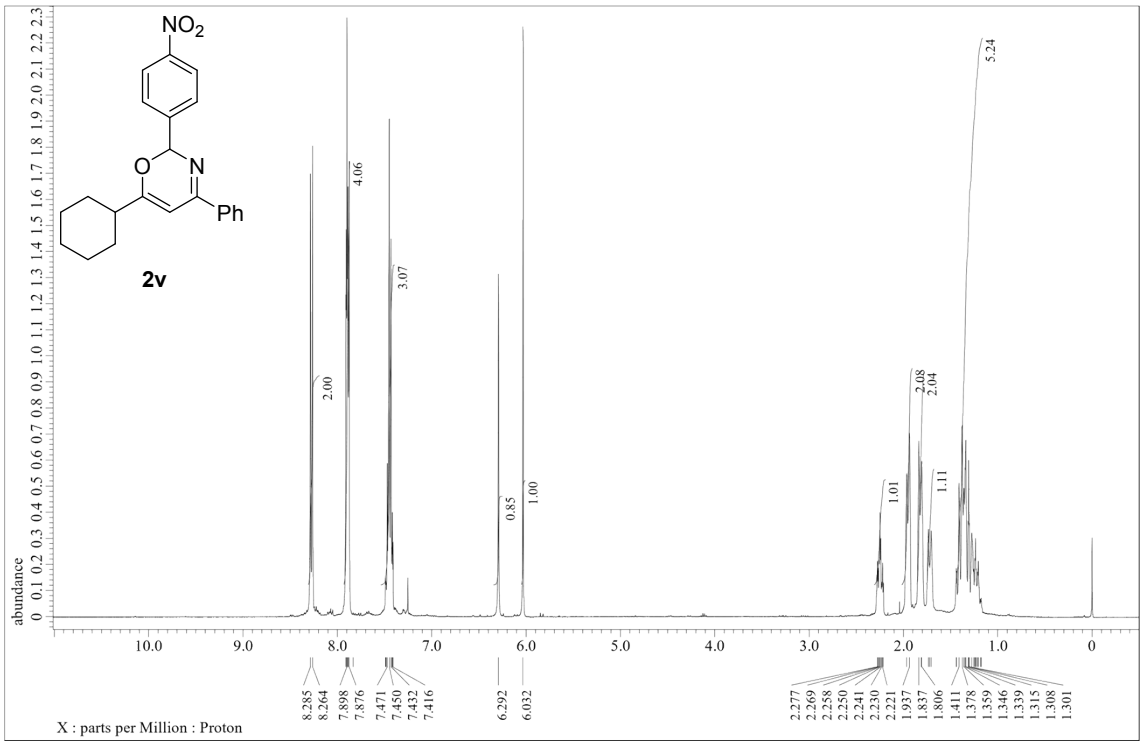

0.2
0.1
0
abundance
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
164.709
163.784
131.318
131.061
128.716
128.649
128.363
127.724
127.133
126.894
126.361
125.007
123.586
101.733
90.654
X : parts per Million : Carbon13

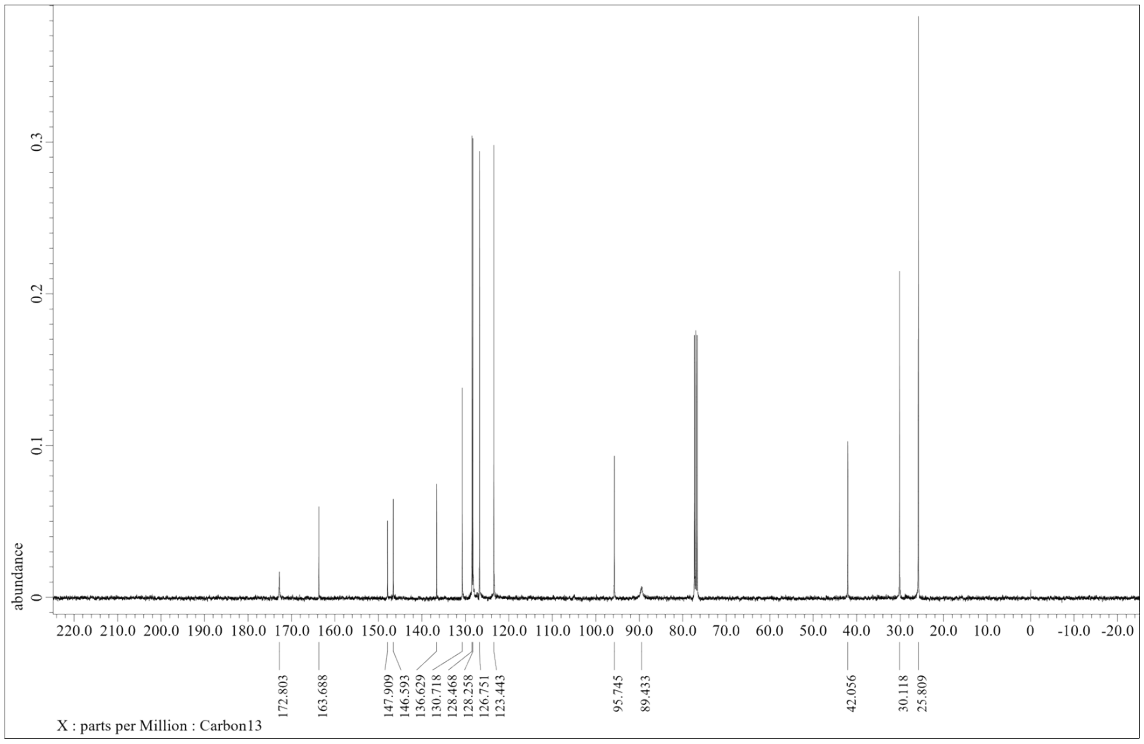

NO2
O
N
Ph
2t
abundance
20.0
10.0
0
9.01
4.09
3.21
2.04
0.91
1.00
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
8.301 8.296 8.291 8.278 8.274 8.268 7.912 7.890 7.469 7.464 7.462 7.457 7.443
6.268 6.101
1.239
X : parts per Million : Proton

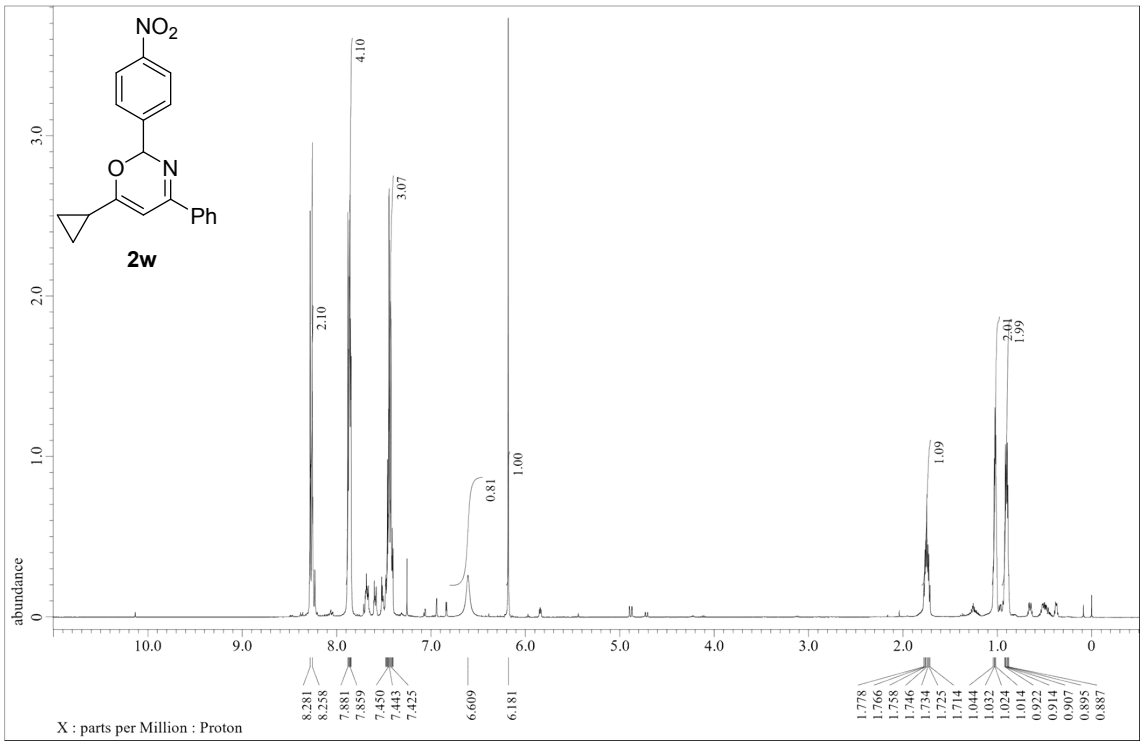

abundance
0.3
0.2
0.1
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
175.616
164.013
147.937
146.593
136.753
130.737
128.496
128.229
126.780
123.462
94.391
89.424
35.849
27.535
X : parts per Million : Carbon13

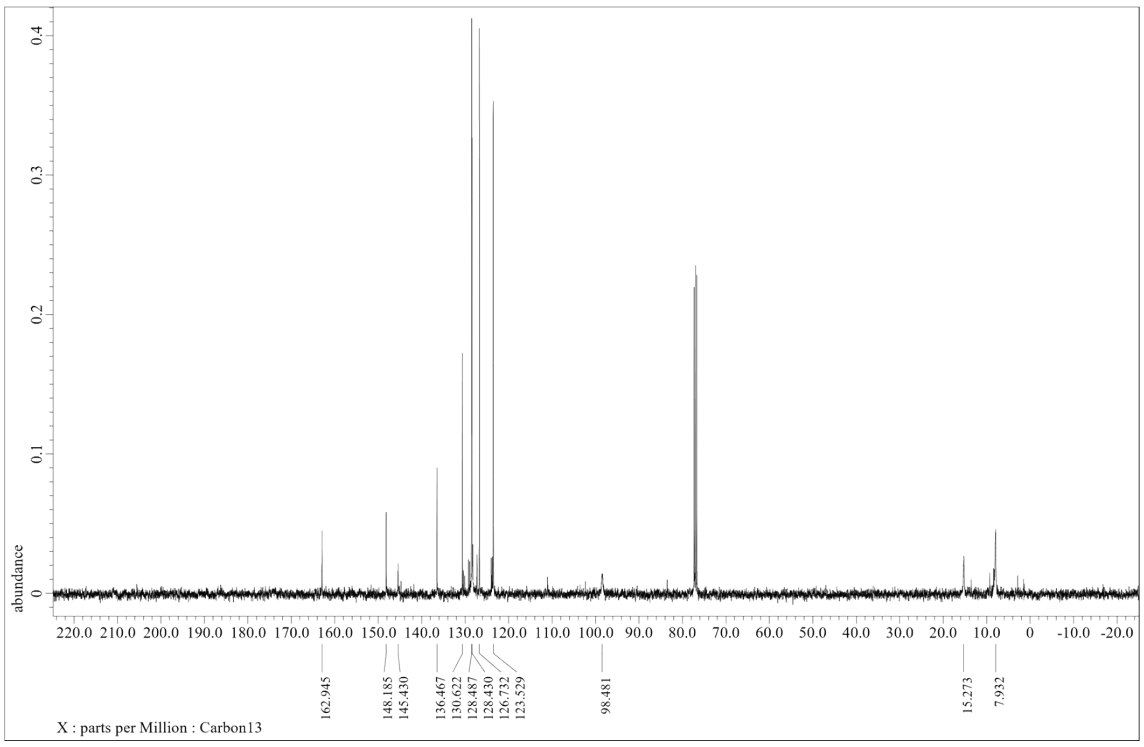

NO2
O
N
Ph
2u
abundance
6.04
4.07
3.28
1.99
0.82
1.00
0.96
8.280
8.258
8.240
7.910
7.897
7.876
7.835
7.487
7.469
7.450
7.432
7.416
7.394
6.332
6.052
2.616
2.599
2.582
2.565
2.548
2.530
2.513
1.222
1.205
X : parts per Million : Proton

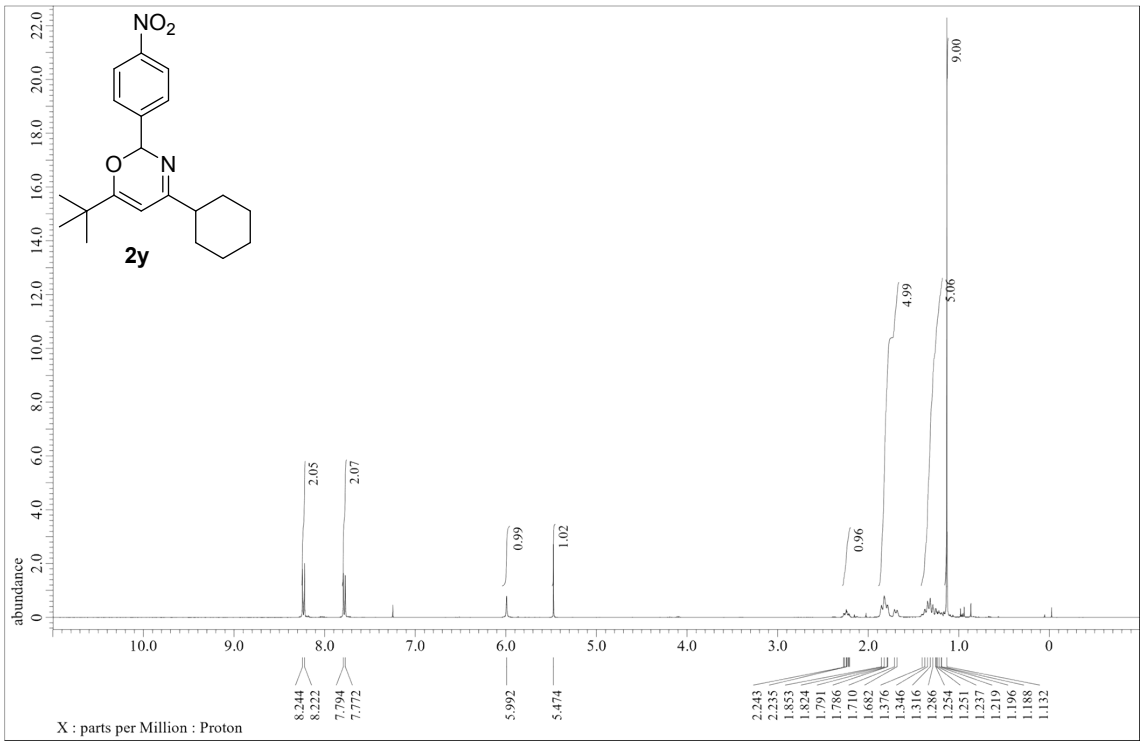

abundance
173.671
163.603
147.909
146.507
136.563
130.718
128.830
128.458
128.220
126.723
123.739
123.414
95.421
89.929
32.540
19.707
X : parts per Million : Carbon13

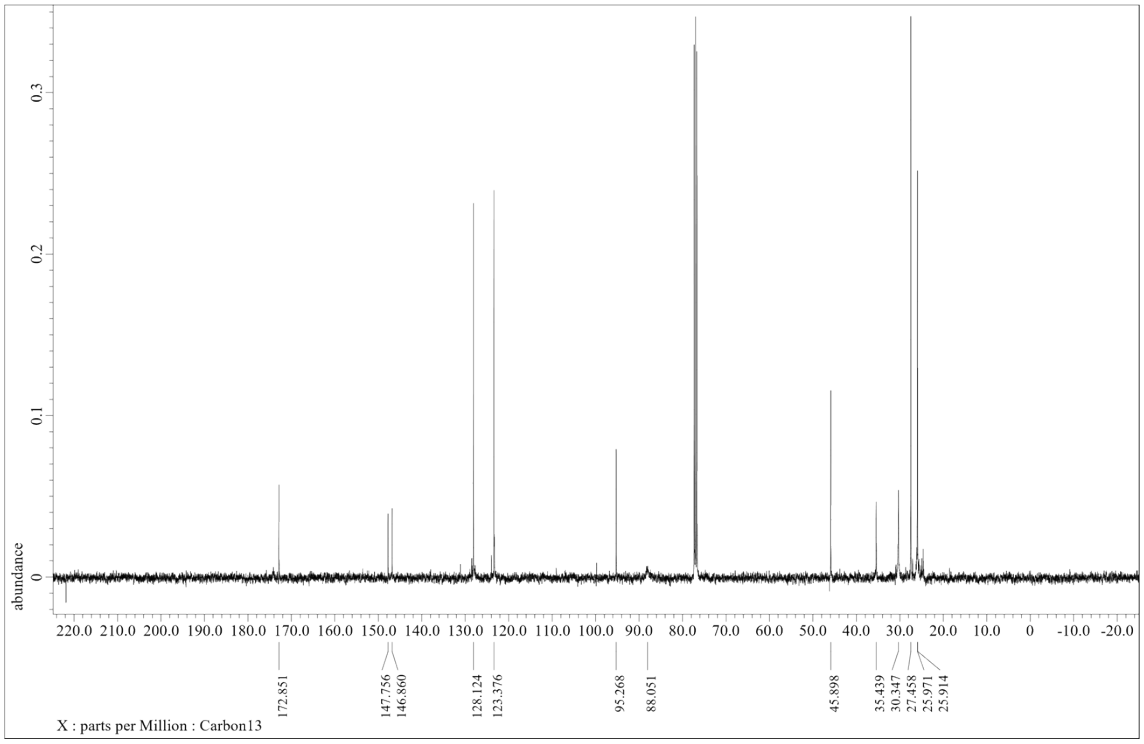

NO2
O
N
Ph
2v
abundance
X : parts per Million : Proton

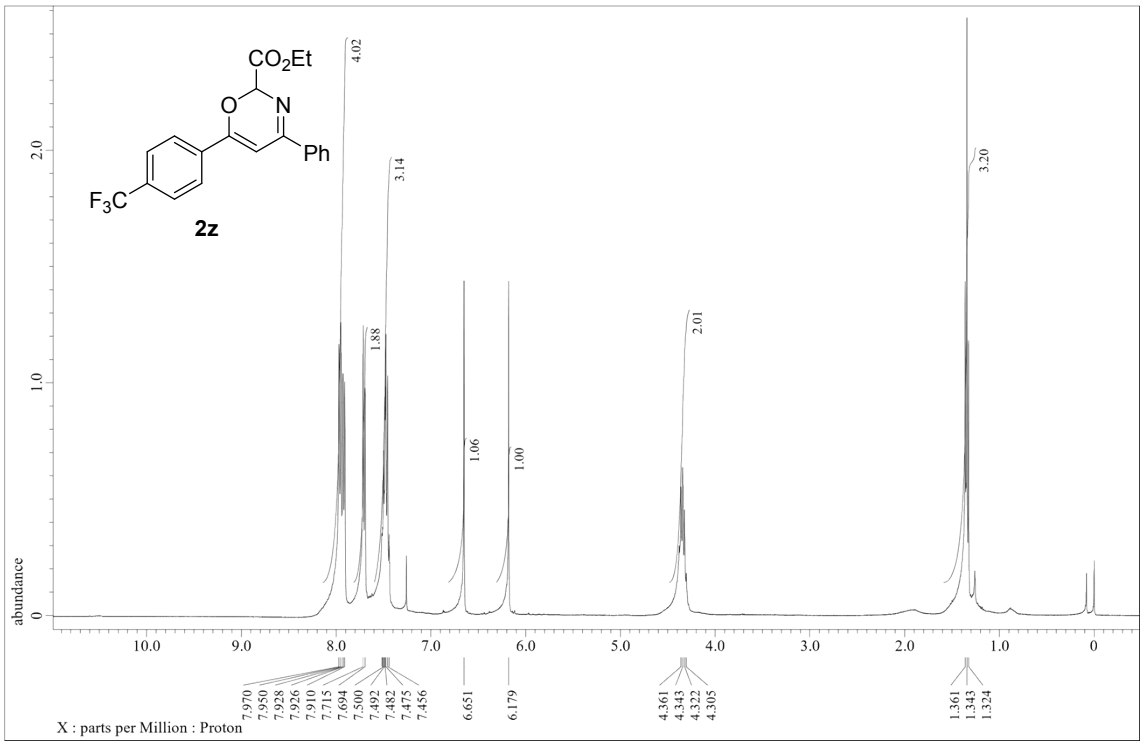

abundance
X : parts per Million : Carbon13

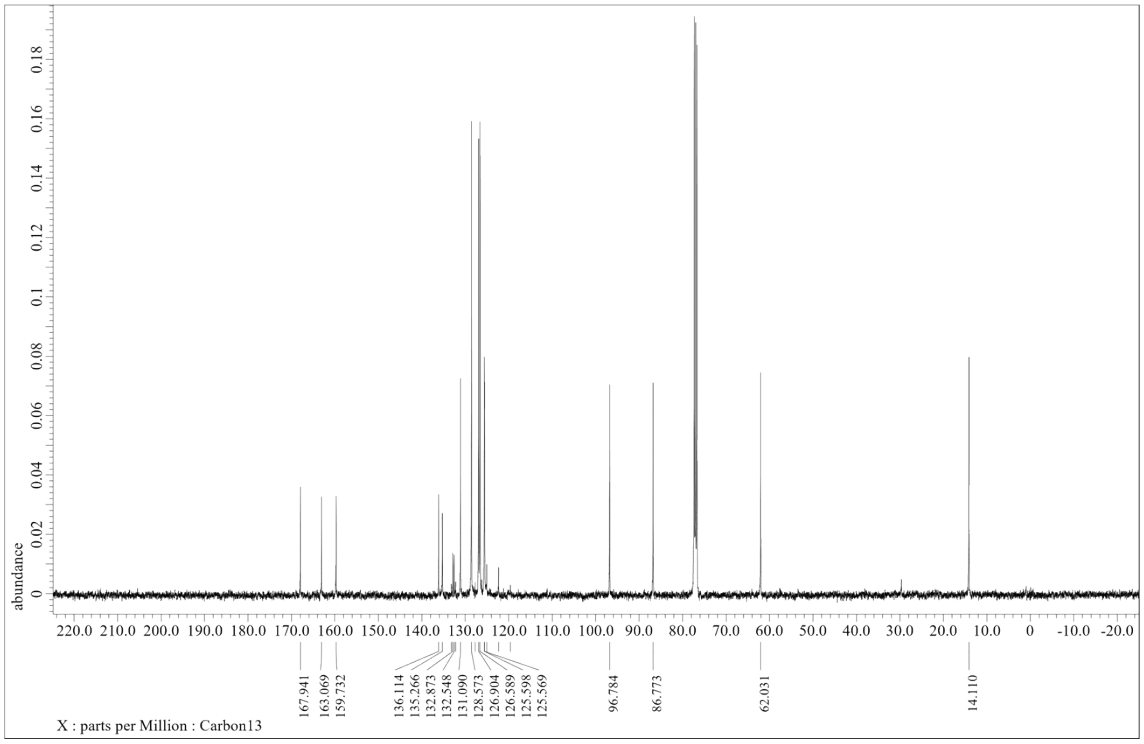

NO2
O
N
Ph
2w
abundance
X : parts per Million : Proton

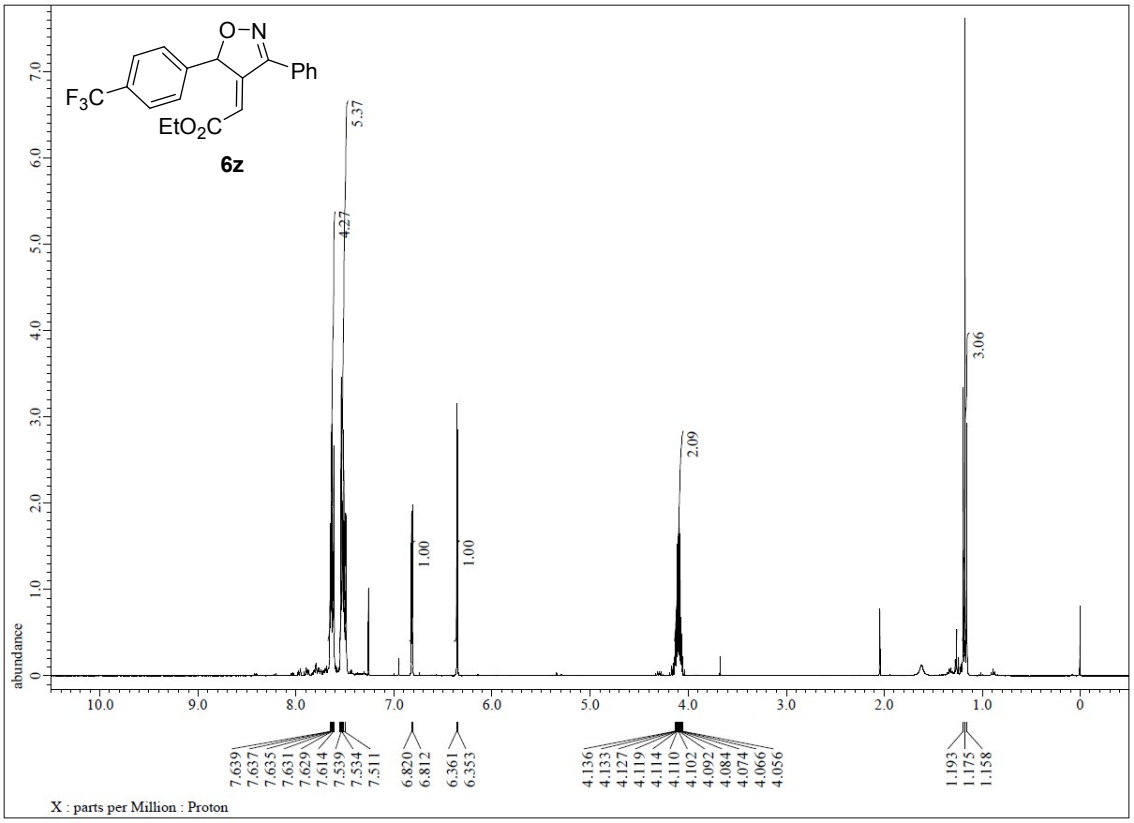

abundance
X : parts per Million : Carbon13

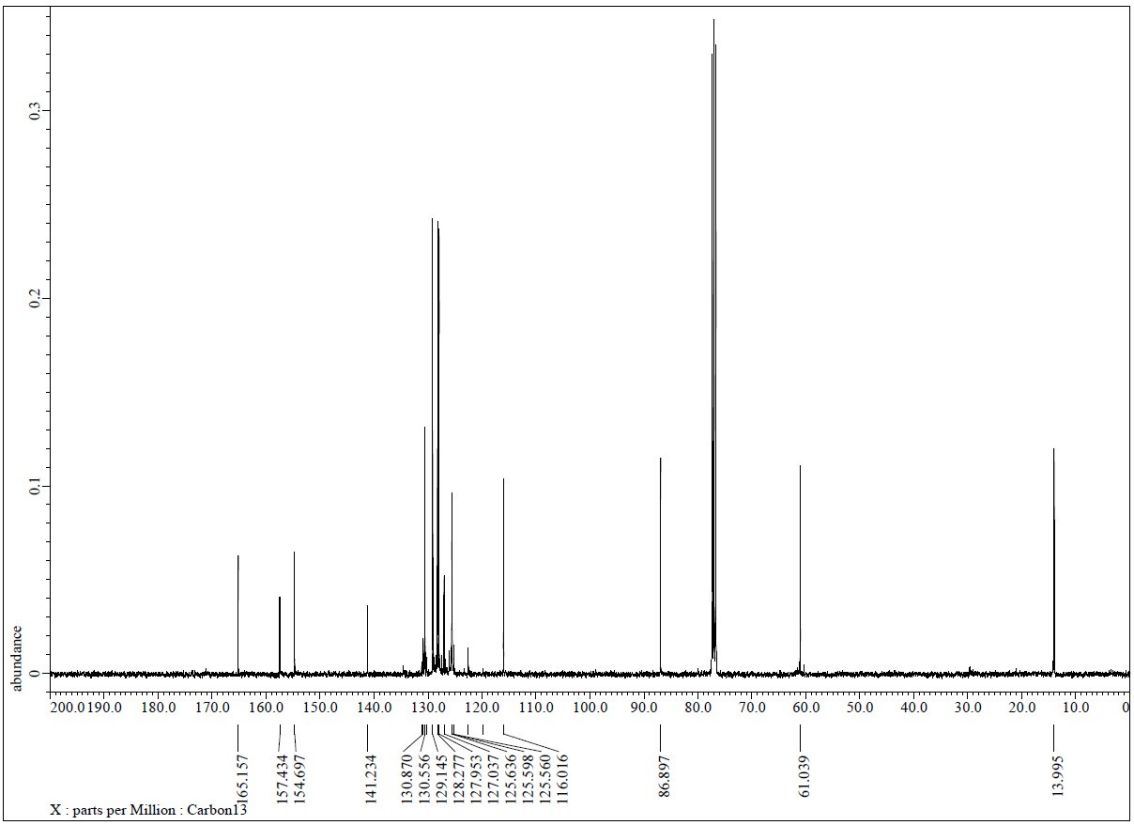

NO2
O
N
2y
abundance
X : parts per Million : Proton
2.05
2.07
0.99
1.02
0.96
4.99
5.06
9.00
8.244
8.222
7.794
7.772
5.992
5.474

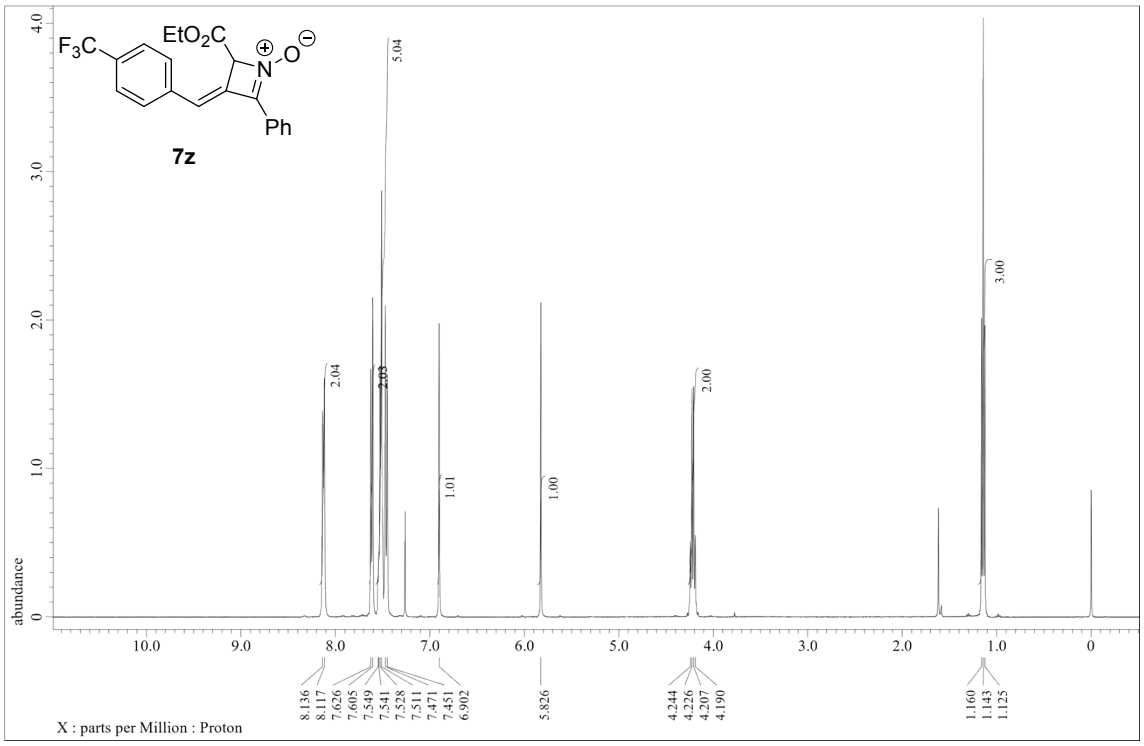

abundance
X : parts per Million : Carbon13
172.851
147.756
146.860
128.124
123.376
95.268
88.051
45.898
35.439
30.347
27.458
25.971
25.914

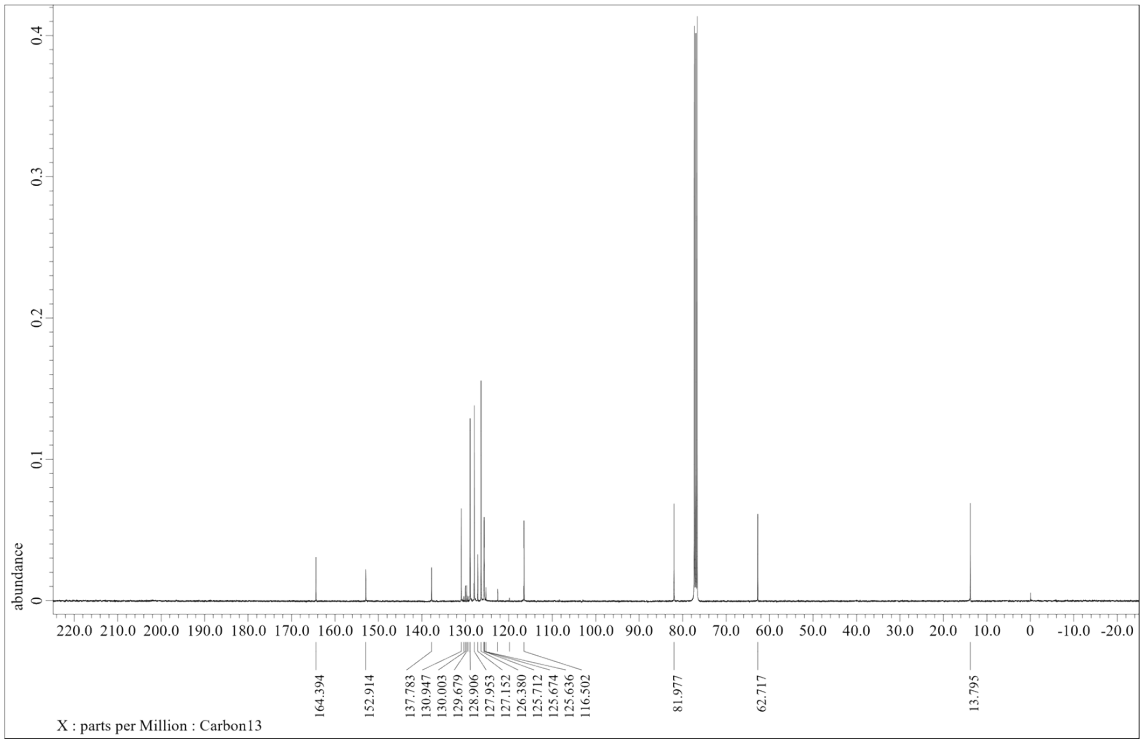

CO2Et
O
N
Ph
F3C
2z
4.02
3.14
1.88
1.06
1.00
2.01
3.20
abundance
X : parts per Million : Proton
7.970
7.950
7.928
7.926
7.910
7.715
7.694
7.500
7.492
7.482
7.475
7.456
6.651
6.179
4.361
4.343
4.322
4.305
1.361
1.343
1.324


abundance
X : parts per Million : Carbon13
167.941
163.069
159.732
136.114
135.266
132.873
132.548
131.090
128.573
126.904
126.589
125.598
125.569
96.784
86.773
62.031
14.110


O–N
Ph
F3C
EtO2C
6z
5.37
4.27
3.06
2.09
1.00
1.00
abundance
X : parts per Million : Proton


abundance
X : parts per Million : Carbon13


F3C
EtO2C
N
O
Ph
7z
5.04
2.04
2.03
1.01
1.00
2.00
3.00
abundance
8.136
8.117
7.626
7.605
7.549
7.541
7.528
7.511
7.471
7.451
6.902
5.826
4.244
4.226
4.207
4.190
1.160
1.143
1.125
X : parts per Million : Proton

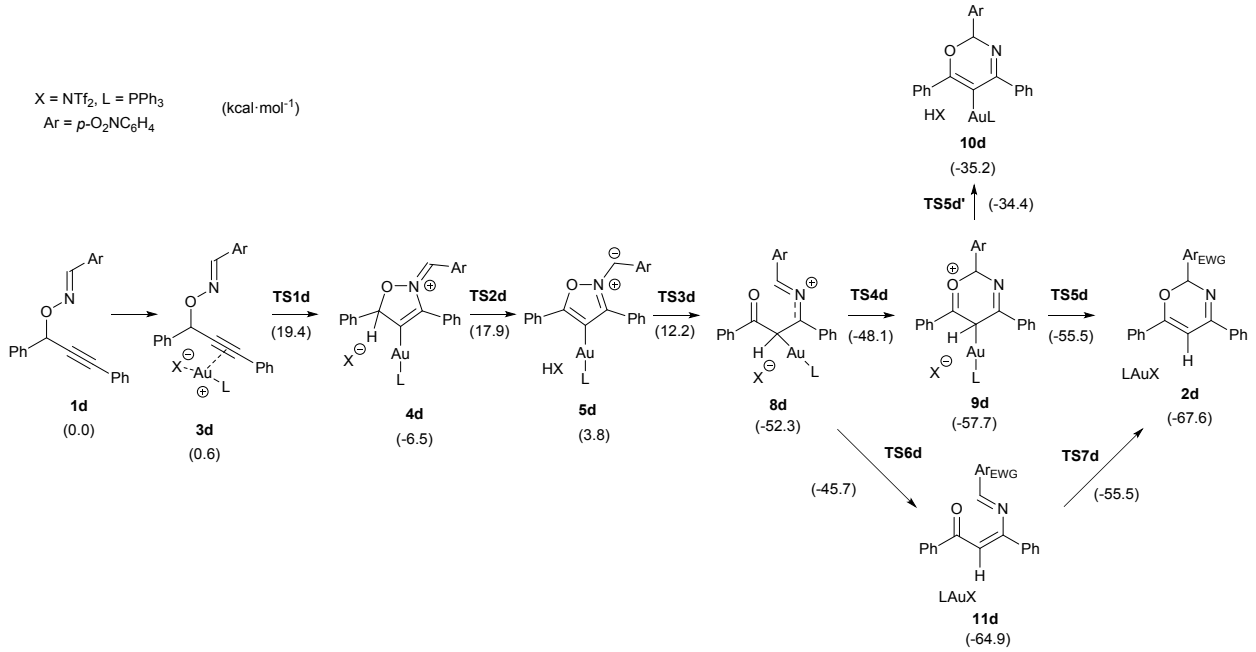

abundance
164.394
152.914
137.783
130.947
130.003
129.679
128.906
127.953
127.152
126.380
125.712
125.674
125.636
116.502
81.977
62.717
13.795
X : parts per Million : Carbon13

13. Computational details

Computations were carried out using the range separated hybrid functional with damped atom—atom dispersion (WB97XD)[1] as implemented in the GAUSSIAN 16 software package.[2] For gold atom the SDD basis set[3] with the associated effective core potential was employed. All other atoms were described with 6-31G** basis with additional diffuse function for phosphorus.[4] Non-specific solvation was introduced by using the SMD continuum model[5] (dichloroethane).

1. J._D. Chai, M. Head_Gordon, *Phys. Chem. Chem. Phys*., 2008, **10**, 6615.
2. Gaussian 16, Revision A.03,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.
3. A. Bergner, M. Dolg, W. Kuechle, H. Stoll, H. Preuss, *Mol. Phys.*, 1993, **80**, 1431.
4. (a) R. Ditchfield, W. J. Hehre, J. A. Pople, *J. Chem. Phys.*,1971, **54**, 724; (b) W. J. Hehre, R. Ditchfield, J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257; (c) P. C. Hariharan, J. A. Pople, *Theor. Chim. Acta*, 1973, **28**, 213; (d) P. C. Hariharan, J. A. Pople, *Mol. Phys.*, 1974, **27**, 209; (e) M. S. Gordon, *Chem. Phys. Lett.*, 1980, **76**, 163.
5. A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378.

Table S16. Computed parameters for the catalytic cycle (wB79XD/SDD(Au)/6-31G**(all others)/SMD(dichloroethane).



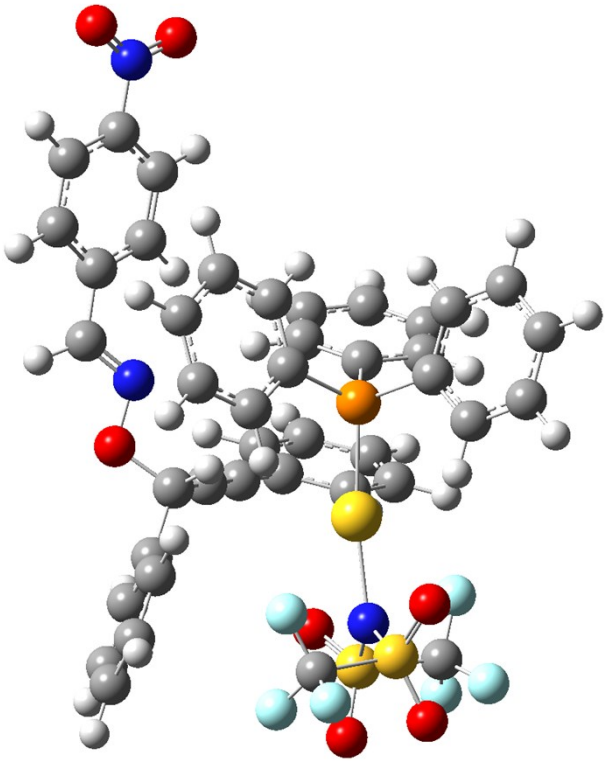
Compound	SCF energy, a.u.	E(ZPVE), a. u.	H, a.u.	G(298), a.u.	Imaginary frequency, cm^{-1} [a]
1d	-1182.587861	-1182.254964	-1182.232209	-1182.312308	
LAuX	-2998.768596	-2998.433171	-2998.399249	-2998.505178	
1d+LAuX	-4181.356457	-4180.688001	-4180.631383	-4180.816749	
3d	-4181.380159	-4180.710182	-4180.651317	-4180.816519	
TS1d	-4181.350308	-4180.680687	-4180.622618	-4180.786556	*i*115.9
4d	-4181.400208	-4180.726737	-4180.669429	-4180.827794	
TS2d	-4181.351487	-4180.68552	-4180.628145	-4180.788979	*i*1527
5d	-4181.37808	-4180.7072	-4180.649292	-4180.811382	
Ts3d	-4181.366161	-4180.699483	-4180.642653	-4180.798043	*i*746.2
8d	-4181.467717	-4180.796189	-4180.737884	-4180.900834	
TS4d	-4181.460614	-4180.789929	-4180.732229	-4180.894059	*i*127.0
9d	-4181.481179	-4180.807038	-4180.749815	-4180.909381	
TS5d	-4181.480864	-4180.807347	-4180.751022	-4180.905876	*i*1010
2d+LAuX	-4181.498059	-4180.823811	-4180.766711	-4180.92523	
TS5d'	-4181.441726	-4180.773304	-4180.716665	-4180.872274	*i*24.9
10d	-4181.445492	-4180.773015	-4180.715689	-4180.873713	
TS for [1,2]-hydrogen shift	-4181.333968	-4180.666868	-4180.609386	-4180.770429	*i*1063
TS6d	-4181.459902	-4180.789284	-4180.732649	-4180.889607	*I*21.4[b]
11d	-1182.693479	-1182.359034	-1182.33603	-1182.415017	
11d+LAuX	-4181.448522	-4180.779043	-4180.723128	-4180.905242	
Ts7d	-1182.679926	-1182.345872	-1182.323879	-1182.400064	*i*345.9

Ts7d+LAuX	-4181.448522	-4180.779043	-4180.723128	-4180.905242	
4t	-4107.647522	-4106.943558	-4106.885176	-4107.045575	
Ts2t	-4107.590913	-4106.8935	-4106.835624	-4106.994801	*i*1446.19
4a	-3976.969198	-3976.299365	-3976.244244	-3976.399443	
Ts2a	-3976.914286	-3976.251026	-3976.196208	-3976.349732	*i*1118
4t complex with pyridine	-4355.87388	-4355.078495	-4355.014743	-4355.18882	[c]
Ts2t-py	-4355.840818	-4355.051261	-4354.986997	-4355.162818	*i*1616

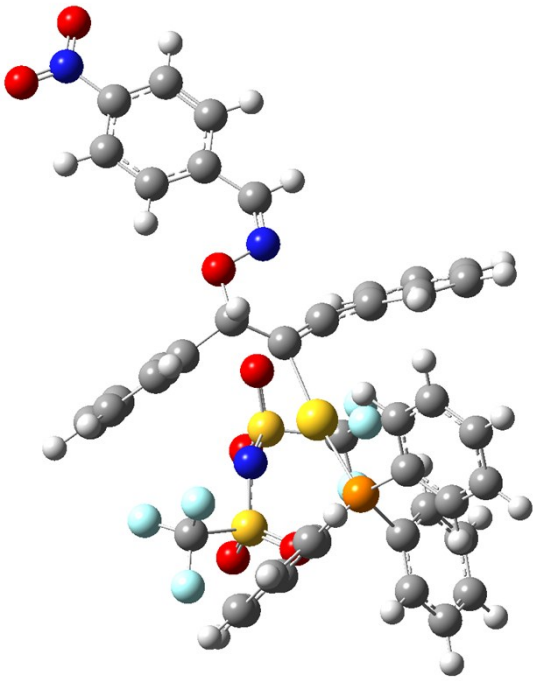
[a] Small imaginary frequency (*i*9.21 cm^{-1}) was neglected; [c] Small imaginary frequency (*i*12.9 cm^{-1}) was neglected. [c] Small imaginary frequency (*i*12.2 cm^{-1}) was neglected.

Figure S4. Geometry of the computed intermediates and transition states

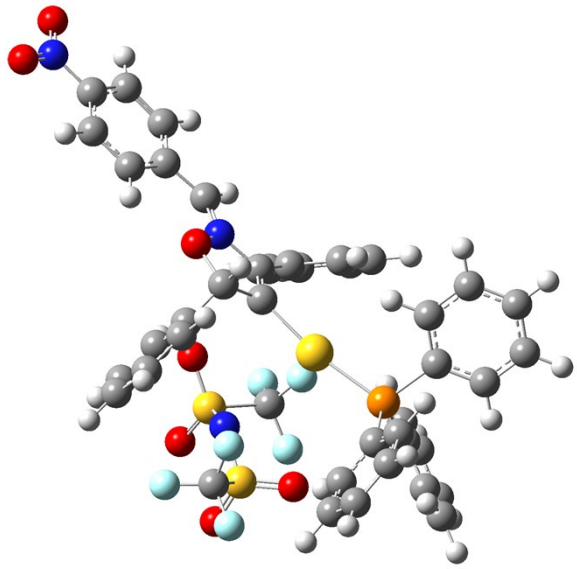
3d



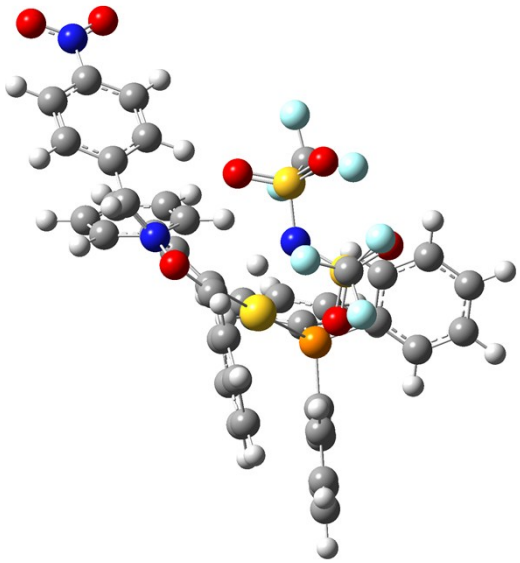
TS1d



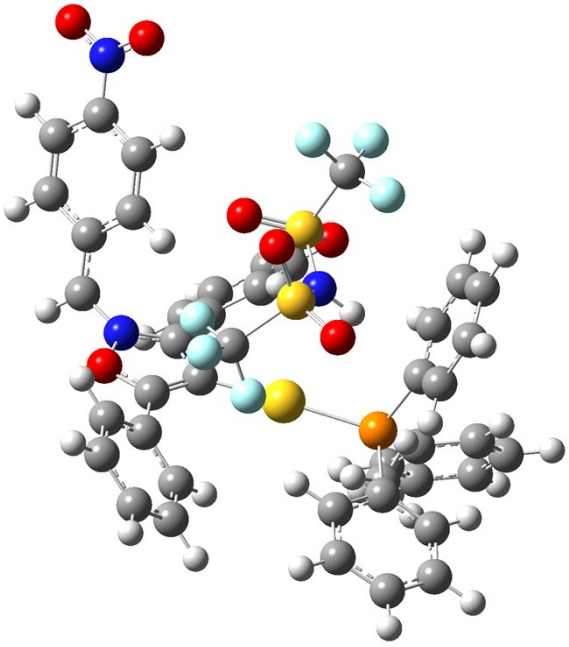
4d



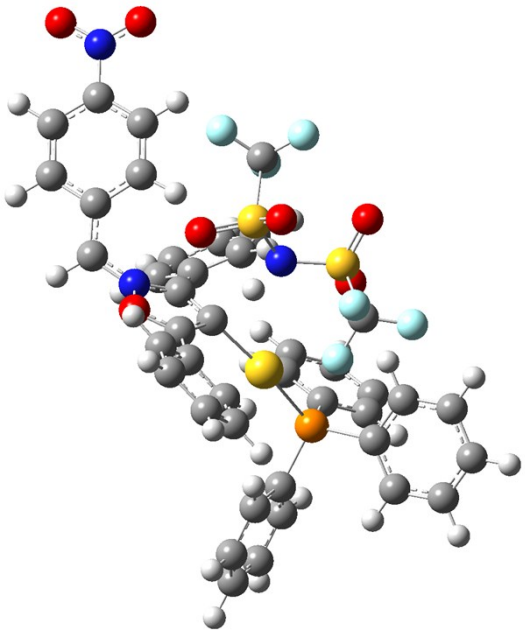
TS2d[a]



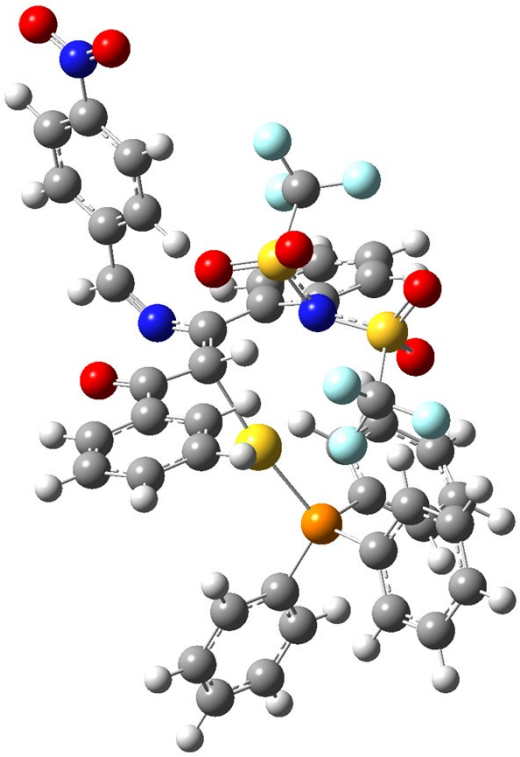
5d[a]



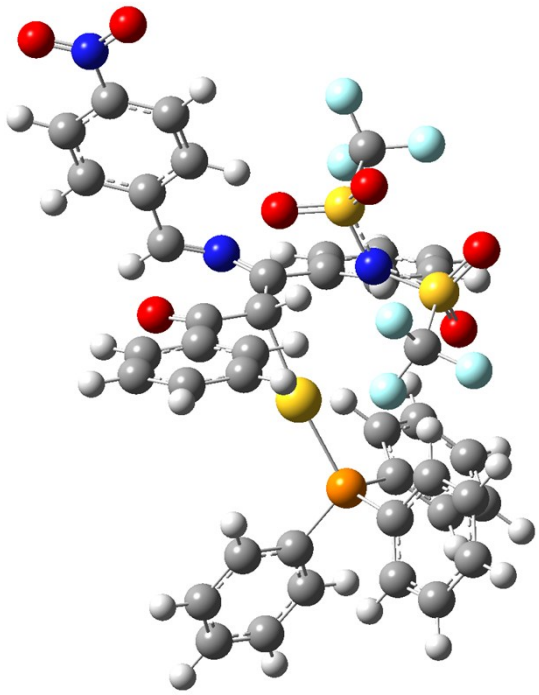
TS3d[a]



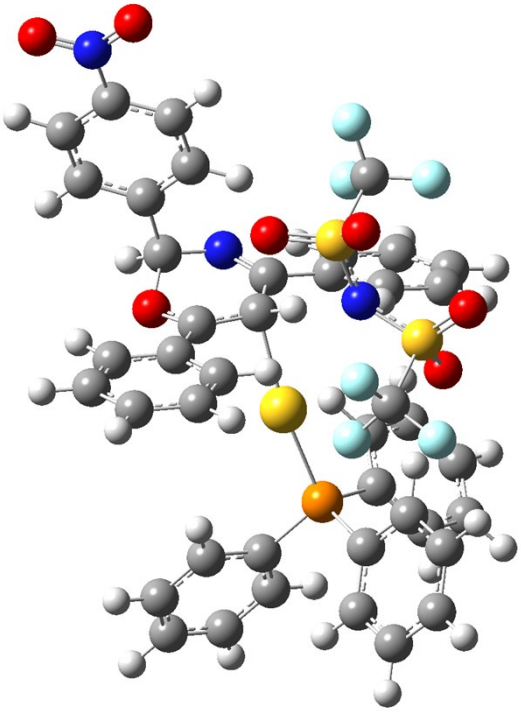
8d[a]



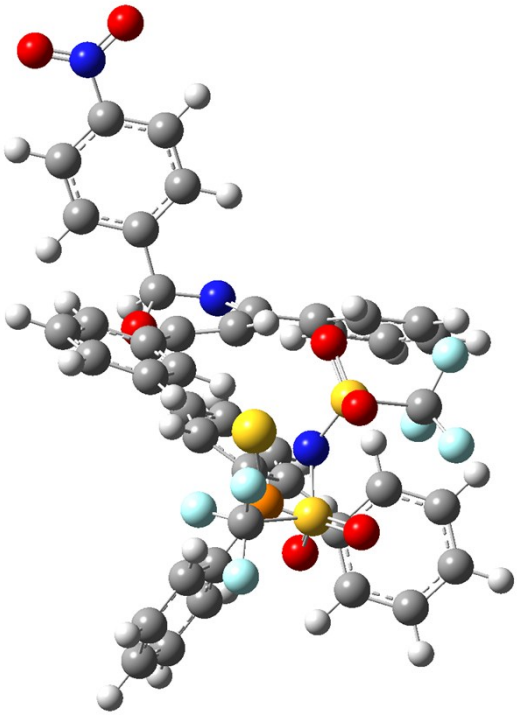
TS4d[a]



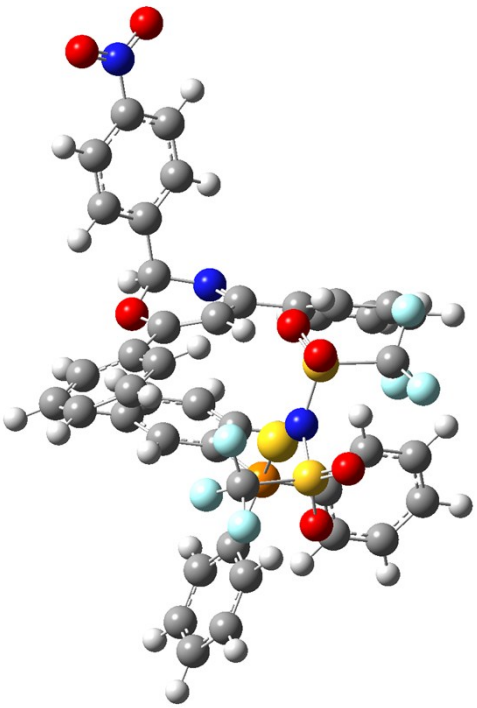
9d[a]



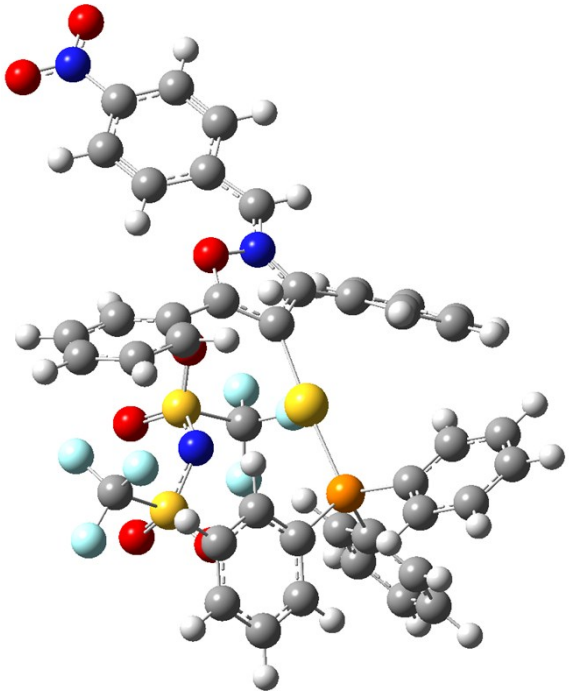
TS5d[a]



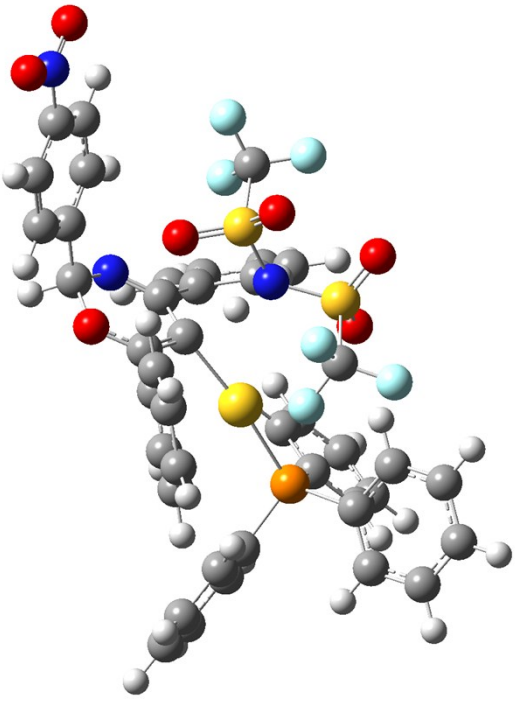
2d[a]



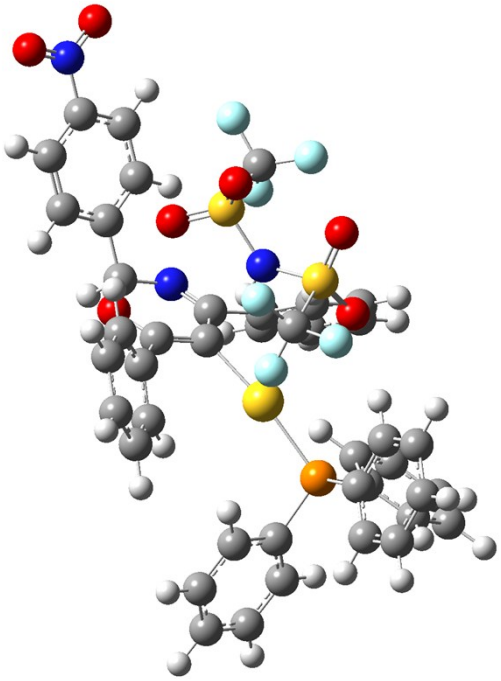
TS for [1,2] hydrogen shift



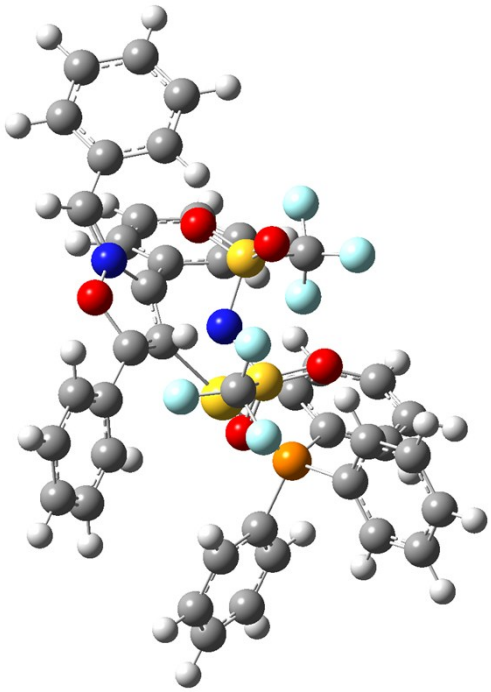
TS5d' [a]



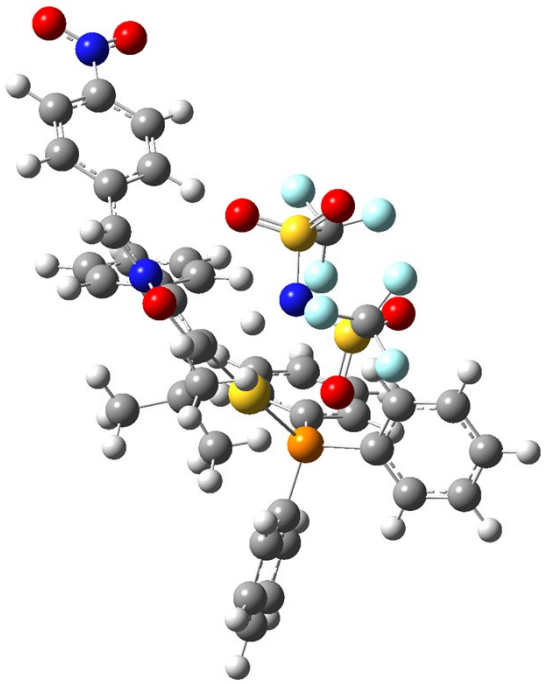
10d[a]



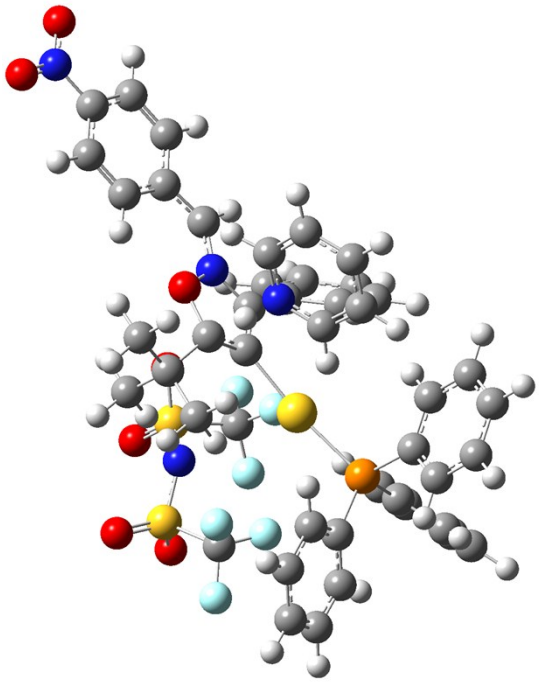
TS2a[a]



TS2t[a]



TS2t-py



[a] The calculated structure was mirror-inverted for clarity.

Cartesian coordinates

1d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.883481	-0.575555	-0.356904
2	6	0	2.737529	-0.220892	-0.504721
3	6	0	5.242562	-0.997204	-0.178172
4	6	0	6.023808	-0.440567	0.844747
5	6	0	5.799257	-1.966878	-1.024574
6	6	0	7.340913	-0.850629	1.014945
7	1	0	5.591568	0.309988	1.498442
8	6	0	7.117420	-2.370347	-0.847272
9	1	0	5.193681	-2.397041	-1.815575
10	6	0	7.889561	-1.814319	0.170920
11	1	0	7.940641	-0.416162	1.808287
12	1	0	7.542908	-3.120804	-1.505787
13	6	0	1.366257	0.255837	-0.693846
14	1	0	1.089839	0.158016	-1.750501
15	6	0	1.208990	1.703918	-0.262395
16	6	0	1.281217	2.040266	1.090874
17	6	0	0.992192	2.699552	-1.211697
18	6	0	1.139210	3.364860	1.487965
19	1	0	1.442628	1.260668	1.829741
20	6	0	0.856979	4.028312	-0.813794
21	1	0	0.927181	2.435668	-2.263756
22	6	0	0.929434	4.362125	0.535415
23	1	0	1.192969	3.621506	2.541428
24	1	0	0.689020	4.800140	-1.558412
25	8	0	0.528959	-0.621862	0.078533
26	7	0	-0.789547	-0.367263	-0.236879
27	6	0	-1.584156	-1.057379	0.484661
28	1	0	-1.208379	-1.741924	1.246509
29	6	0	-3.036808	-0.941925	0.297256
30	6	0	-3.593451	-0.041179	-0.622314
31	6	0	-3.878244	-1.753702	1.065304
32	6	0	-4.966569	0.044998	-0.773867
33	1	0	-2.943491	0.592411	-1.214947
34	6	0	-5.256651	-1.677665	0.923188
35	1	0	-3.451416	-2.451126	1.778823
36	6	0	-5.777192	-0.777362	0.003393
37	1	0	-5.409612	0.736556	-1.479099
38	1	0	-5.917112	-2.301563	1.511694
39	1	0	8.918662	-2.131791	0.306489
40	1	0	0.819982	5.396358	0.846680
41	7	0	-7.229204	-0.689021	-0.153624
42	8	0	-7.929041	-1.415309	0.538799
43	8	0	-7.672700	0.106857	-0.969978

LAuX

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	-0.182154	-0.019695	-0.006343
2	15	0	2.099594	-0.000122	-0.005451
3	6	0	2.818329	-0.921241	-1.401982
4	6	0	2.149838	-0.911342	-2.630889

5	6	0	4.032112	-1.603405	-1.276581
6	6	0	2.697001	-1.570875	-3.725762
7	1	0	1.198378	-0.396046	-2.730416
8	6	0	4.573584	-2.263526	-2.375469
9	1	0	4.552799	-1.624487	-0.323961
10	6	0	3.908156	-2.246701	-3.598554
11	1	0	2.170885	-1.564258	-4.674637
12	1	0	5.514311	-2.794763	-2.273116
13	1	0	4.330776	-2.766769	-4.452420
14	6	0	2.769342	1.691465	-0.103482
15	6	0	2.108333	2.711711	0.590750
16	6	0	3.932241	1.980146	-0.822417
17	6	0	2.613611	4.006416	0.570711
18	1	0	1.197882	2.495821	1.143542
19	6	0	4.430409	3.279936	-0.842066
20	1	0	4.446929	1.196816	-1.370073
21	6	0	3.773691	4.291162	-0.146363
22	1	0	2.095763	4.793652	1.108677
23	1	0	5.331119	3.501490	-1.405461
24	1	0	4.162454	5.304345	-0.167421
25	6	0	2.811630	-0.740551	1.499748
26	6	0	3.934745	-0.194802	2.125918
27	6	0	2.226721	-1.905238	2.010233
28	6	0	4.469997	-0.814255	3.252264
29	1	0	4.389301	0.713219	1.742618
30	6	0	2.768730	-2.521471	3.131677
31	1	0	1.345810	-2.327524	1.533636
32	6	0	3.889948	-1.975695	3.753552
33	1	0	5.339598	-0.384606	3.739036
34	1	0	2.310250	-3.422884	3.524933
35	1	0	4.307788	-2.453947	4.633778
36	7	0	-2.305475	-0.007468	0.005672
37	16	0	-3.091926	-1.180233	-0.845919
38	8	0	-4.462560	-0.843853	-1.162330
39	8	0	-2.177820	-1.646698	-1.872328
40	16	0	-3.068964	1.179428	0.858980
41	8	0	-4.432347	0.850327	1.212024
42	8	0	-2.130420	1.656992	1.858176
43	6	0	-3.153458	-2.544956	0.409729
44	6	0	-3.155581	2.531110	-0.409466
45	9	0	-3.775870	-2.134163	1.504339
46	9	0	-3.800085	-3.578980	-0.110736
47	9	0	-1.915182	-2.920682	0.729131
48	9	0	-3.793563	3.569251	0.114399
49	9	0	-3.797950	2.110795	-1.488885
50	9	0	-1.923606	2.903931	-0.753601

3d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.323587	0.640311	-2.852847
2	6	0	-0.459537	-0.489840	-2.446398
3	6	0	-0.163982	2.010854	-3.234154
4	6	0	-0.886717	2.558168	-4.302306
5	6	0	0.690090	2.829639	-2.482582
6	6	0	-0.758176	3.909182	-4.606030
7	1	0	-1.550648	1.924051	-4.881054
8	6	0	0.814384	4.177741	-2.794498
9	1	0	1.249100	2.395859	-1.660808
10	6	0	0.088493	4.721338	-3.853102

11	1	0	-1.322324	4.329785	-5.432589
12	1	0	1.477163	4.805141	-2.206583
13	6	0	-0.588789	-1.798672	-1.800404
14	1	0	-0.618079	-1.625630	-0.719667
15	6	0	0.542791	-2.753457	-2.103912
16	6	0	1.150205	-2.792165	-3.359098
17	6	0	0.963286	-3.632842	-1.105277
18	6	0	2.172193	-3.702698	-3.610912
19	1	0	0.832974	-2.099665	-4.133246
20	6	0	1.985016	-4.543568	-1.357093
21	1	0	0.493392	-3.595939	-0.126356
22	6	0	2.590589	-4.578802	-2.611013
23	1	0	2.646548	-3.724325	-4.587003
24	1	0	2.315683	-5.215435	-0.571545
25	8	0	-1.807258	-2.471482	-2.162870
26	7	0	-2.883803	-1.755878	-1.679470
27	6	0	-3.960213	-2.439972	-1.729470
28	1	0	-3.959510	-3.474112	-2.076294
29	6	0	-5.218509	-1.841759	-1.262000
30	6	0	-5.393142	-0.452762	-1.213695
31	6	0	-6.242718	-2.684040	-0.816363
32	6	0	-6.555542	0.091370	-0.693160
33	1	0	-4.615920	0.199173	-1.593167
34	6	0	-7.413927	-2.153576	-0.293586
35	1	0	-6.114419	-3.760746	-0.862288
36	6	0	-7.546652	-0.771434	-0.234729
37	1	0	-6.699857	1.163418	-0.646596
38	1	0	-8.209339	-2.794699	0.064666
39	79	0	1.394952	0.236605	0.709077
40	15	0	-0.678542	0.794050	1.499527
41	6	0	-0.566315	1.492205	3.182219
42	6	0	0.610166	1.345591	3.922312
43	6	0	-1.671264	2.136275	3.752378
44	6	0	0.680645	1.840316	5.222962
45	1	0	1.471799	0.847391	3.485204
46	6	0	-1.594428	2.629838	5.049320
47	1	0	-2.587641	2.260327	3.182613
48	6	0	-0.418762	2.481734	5.785506
49	1	0	1.597711	1.725013	5.791766
50	1	0	-2.452083	3.131108	5.486375
51	1	0	-0.361568	2.869158	6.797965
52	6	0	-1.495881	2.070796	0.490078
53	6	0	-2.364188	1.711836	-0.542739
54	6	0	-1.162284	3.416219	0.683902
55	6	0	-2.911684	2.694763	-1.362368
56	1	0	-2.599222	0.667904	-0.723299
57	6	0	-1.708828	4.392360	-0.142390
58	1	0	-0.479906	3.704065	1.478328
59	6	0	-2.585296	4.033303	-1.164757
60	1	0	-3.581557	2.409203	-2.167619
61	1	0	-1.445616	5.434107	0.010180
62	1	0	-3.004329	4.796170	-1.813161
63	6	0	-1.832202	-0.611137	1.639403
64	6	0	-3.212684	-0.414842	1.757848
65	6	0	-1.313147	-1.909666	1.679245
66	6	0	-4.061096	-1.508252	1.891503
67	1	0	-3.630724	0.586413	1.729782
68	6	0	-2.166696	-3.001346	1.810932
69	1	0	-0.240932	-2.069356	1.595241
70	6	0	-3.540969	-2.801057	1.910782
71	1	0	-5.132428	-1.350295	1.965781
72	1	0	-1.756687	-4.006012	1.829148
73	1	0	-4.209340	-3.651509	2.002019
74	7	0	3.453713	-0.194081	0.262531
75	16	0	4.106441	0.255236	-1.179456

76	8	0	5.331095	-0.447452	-1.503093
77	8	0	3.024378	0.335588	-2.140471
78	16	0	4.345337	-0.834223	1.490369
79	8	0	5.771835	-0.628680	1.343876
80	8	0	3.681754	-0.502907	2.739630
81	7	0	-8.775616	-0.203049	0.320274
82	8	0	-9.644610	-0.974211	0.702295
83	8	0	-8.871063	1.015065	0.376697
84	1	0	3.393312	-5.282943	-2.806972
85	1	0	0.184140	5.775803	-4.092755
86	6	0	4.585349	2.017298	-0.841911
87	6	0	4.052549	-2.648999	1.250400
88	9	0	5.431093	2.079659	0.176620
89	9	0	5.156077	2.517852	-1.928919
90	9	0	3.502182	2.734286	-0.546991
91	9	0	4.782939	-3.317031	2.133968
92	9	0	4.400845	-3.005542	0.024082
93	9	0	2.766690	-2.928109	1.447183

TS1d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.349602	1.769793	0.052018
2	6	0	1.117342	0.815395	-0.736718
3	6	0	1.321871	2.846608	0.976226
4	6	0	1.861880	2.679246	2.261820
5	6	0	0.737241	4.068078	0.599927
6	6	0	1.815469	3.733463	3.162082
7	1	0	2.293730	1.722002	2.533776
8	6	0	0.683504	5.109396	1.515362
9	1	0	0.322933	4.177742	-0.397317
10	6	0	1.224883	4.942158	2.790689
11	1	0	2.228335	3.612059	4.157856
12	1	0	0.223792	6.051852	1.237344
13	6	0	2.048091	0.126775	-1.680073
14	1	0	1.882737	0.552327	-2.677207
15	6	0	1.905738	-1.374617	-1.730394
16	6	0	2.230460	-2.135738	-0.605627
17	6	0	1.470371	-2.001152	-2.895466
18	6	0	2.133117	-3.520395	-0.657218
19	1	0	2.540639	-1.641714	0.310274
20	6	0	1.359647	-3.390536	-2.939918
21	1	0	1.223292	-1.404498	-3.769822
22	6	0	1.697881	-4.149760	-1.823743
23	1	0	2.383412	-4.109612	0.218870
24	1	0	1.018463	-3.876464	-3.848789
25	8	0	3.425606	0.381436	-1.306129
26	7	0	3.584753	1.529339	-0.604542
27	6	0	4.784658	1.850686	-0.298195
28	1	0	4.829884	2.773602	0.275551
29	6	0	6.068774	1.193000	-0.584846
30	6	0	6.205939	-0.043673	-1.235443
31	6	0	7.219544	1.867990	-0.147068
32	6	0	7.466111	-0.585915	-1.446797
33	1	0	5.334634	-0.588265	-1.570231
34	6	0	8.482313	1.337023	-0.354773
35	1	0	7.121835	2.821267	0.363043
36	6	0	8.581912	0.113646	-1.006099
37	1	0	7.582042	-1.540129	-1.945088
38	1	0	9.371793	1.855486	-0.020079
39	79	0	-0.983535	0.586514	-0.713818

40	15	0	-3.288258	0.685307	-1.040055
41	6	0	-3.701174	2.164294	-2.032413
42	6	0	-2.731215	2.716437	-2.876224
43	6	0	-4.982315	2.724787	-1.995056
44	6	0	-3.040158	3.813263	-3.676161
45	1	0	-1.733521	2.285709	-2.906882
46	6	0	-5.285520	3.824275	-2.791837
47	1	0	-5.744474	2.308433	-1.343538
48	6	0	-4.316474	4.368472	-3.632941
49	1	0	-2.281841	4.235099	-4.328209
50	1	0	-6.280308	4.256626	-2.754367
51	1	0	-4.556641	5.226850	-4.252656
52	6	0	-3.971005	-0.723836	-1.978578
53	6	0	-4.067646	-1.970370	-1.348737
54	6	0	-4.330655	-0.595047	-3.322502
55	6	0	-4.524732	-3.074024	-2.060134
56	1	0	-3.789945	-2.073725	-0.304032
57	6	0	-4.783874	-1.706380	-4.030098
58	1	0	-4.262010	0.365998	-3.822027
59	6	0	-4.881937	-2.944403	-3.401417
60	1	0	-4.598034	-4.036893	-1.565433
61	1	0	-5.062873	-1.599832	-5.073688
62	1	0	-5.235939	-3.808606	-3.954971
63	6	0	-4.274660	0.829321	0.482864
64	6	0	-5.576053	0.328627	0.577916
65	6	0	-3.706951	1.497753	1.571673
66	6	0	-6.298337	0.494490	1.756581
67	1	0	-6.025504	-0.196734	-0.258925
68	6	0	-4.432474	1.662762	2.746080
69	1	0	-2.692439	1.878746	1.504793
70	6	0	-5.728132	1.158944	2.839897
71	1	0	-7.306836	0.099666	1.828216
72	1	0	-3.980301	2.172732	3.590694
73	1	0	-6.291544	1.278769	3.760024
74	7	0	-0.210125	-1.814074	1.837600
75	16	0	0.681881	-1.283031	3.043915
76	8	0	0.830662	-2.176532	4.183764
77	8	0	1.880442	-0.673278	2.478406
78	16	0	-1.564156	-2.658724	1.995333
79	8	0	-1.632918	-3.570949	3.130067
80	8	0	-2.742909	-1.843015	1.708855
81	7	0	9.911118	-0.459149	-1.233655
82	8	0	10.879910	0.156272	-0.813590
83	8	0	9.983243	-1.522124	-1.832879
84	1	0	1.616341	-5.231891	-1.857594
85	1	0	1.183485	5.760858	3.502443
86	6	0	-0.297786	0.140075	3.712867
87	6	0	-1.372856	-3.736417	0.506803
88	9	0	-1.419717	-0.306068	4.276008
89	9	0	0.417996	0.788308	4.629023
90	9	0	-0.623797	0.993995	2.743502
91	9	0	-2.511991	-4.410227	0.334889
92	9	0	-0.388047	-4.607450	0.687135
93	9	0	-1.134715	-3.017213	-0.585814

4d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.060940	-1.088698	-0.260835
2	6	0	1.208179	-0.588203	0.646434
3	6	0	1.818105	-1.819381	-1.519846

4	6	0	2.328233	-1.362122	-2.739457
5	6	0	1.003299	-2.956688	-1.496372
6	6	0	2.028006	-2.037555	-3.917998
7	1	0	2.920809	-0.453549	-2.768895
8	6	0	0.693979	-3.620789	-2.679195
9	1	0	0.608789	-3.312533	-0.549296
10	6	0	1.208462	-3.163756	-3.890936
11	1	0	2.417857	-1.669450	-4.861407
12	1	0	0.055358	-4.498186	-2.652663
13	6	0	2.015003	-0.026495	1.773248
14	1	0	1.898702	-0.649561	2.667626
15	6	0	1.809971	1.424214	2.119489
16	6	0	2.046119	2.412325	1.161558
17	6	0	1.397650	1.779569	3.401858
18	6	0	1.878563	3.750524	1.494011
19	1	0	2.334195	2.132319	0.152262
20	6	0	1.217400	3.122595	3.729386
21	1	0	1.220863	1.006153	4.144792
22	6	0	1.463976	4.107550	2.777637
23	1	0	2.054326	4.516722	0.745748
24	1	0	0.892920	3.396448	4.728494
25	8	0	3.419390	-0.193485	1.349526
26	7	0	3.415323	-0.866126	0.179569
27	6	0	4.524191	-1.240221	-0.366676
28	1	0	4.386499	-1.797901	-1.285563
29	6	0	5.881682	-1.013350	0.101266
30	6	0	6.244279	-0.187912	1.179489
31	6	0	6.882155	-1.680566	-0.627749
32	6	0	7.580444	-0.044347	1.522212
33	1	0	5.497367	0.349069	1.745092
34	6	0	8.217044	-1.546556	-0.285922
35	1	0	6.608270	-2.310359	-1.467707
36	6	0	8.540388	-0.728110	0.788657
37	1	0	7.874000	0.590680	2.348240
38	1	0	8.992494	-2.060249	-0.839241
39	79	0	-0.838205	-0.735154	0.631922
40	15	0	-3.117565	-1.272842	0.751429
41	6	0	-3.331762	-3.034830	1.192462
42	6	0	-2.300453	-3.708583	1.855304
43	6	0	-4.524786	-3.708936	0.909525
44	6	0	-2.461353	-5.039306	2.233052
45	1	0	-1.370424	-3.190116	2.074474
46	6	0	-4.680726	-5.039280	1.285063
47	1	0	-5.332289	-3.197510	0.394065
48	6	0	-3.650214	-5.705279	1.946849
49	1	0	-1.655759	-5.554891	2.746306
50	1	0	-5.607711	-5.556953	1.059407
51	1	0	-3.774036	-6.744200	2.236504
52	6	0	-4.035230	-0.350808	2.033676
53	6	0	-4.232402	1.023751	1.853392
54	6	0	-4.475111	-0.965132	3.208552
55	6	0	-4.867228	1.771456	2.838536
56	1	0	-3.898491	1.501246	0.937263
57	6	0	-5.106959	-0.209079	4.194254
58	1	0	-4.329237	-2.029762	3.361261
59	6	0	-5.303629	1.156718	4.011485
60	1	0	-5.016502	2.835993	2.689762
61	1	0	-5.447059	-0.692722	5.104666
62	1	0	-5.796326	1.742556	4.781358
63	6	0	-4.048404	-1.073046	-0.802463
64	6	0	-5.380881	-0.656420	-0.836992
65	6	0	-3.388118	-1.385609	-1.994858
66	6	0	-6.041868	-0.545740	-2.057907
67	1	0	-5.903931	-0.409387	0.081474
68	6	0	-4.051869	-1.275938	-3.211159

69	1	0	-2.350349	-1.704528	-1.972260
70	6	0	-5.379056	-0.852004	-3.243816
71	1	0	-7.075446	-0.214972	-2.080705
72	1	0	-3.528074	-1.508533	-4.132977
73	1	0	-5.895276	-0.756251	-4.194030
74	7	0	-0.462872	2.368609	-1.206033
75	16	0	0.435644	2.311033	-2.517473
76	8	0	0.396424	3.482785	-3.381960
77	8	0	1.737012	1.768101	-2.146002
78	16	0	-1.918094	3.028589	-1.106531
79	8	0	-2.153613	4.210464	-1.927233
80	8	0	-2.971267	2.015899	-1.060535
81	7	0	9.952340	-0.577491	1.160413
82	8	0	10.783455	-1.184122	0.501758
83	8	0	10.219552	0.145104	2.108402
84	1	0	1.326380	5.154305	3.030844
85	1	0	0.968640	-3.683373	-4.813462
86	6	0	-0.369990	0.985079	-3.527641
87	6	0	-1.800027	3.652256	0.628991
88	9	0	-1.576740	1.394488	-3.921515
89	9	0	0.368949	0.727467	-4.604663
90	9	0	-0.513880	-0.134012	-2.825069
91	9	0	-3.010545	4.075364	1.000698
92	9	0	-0.953984	4.672498	0.698518
93	9	0	-1.409891	2.695824	1.466550

TS2d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.936256	-0.138970	-1.420919
2	6	0	-0.607846	0.254984	-1.409511
3	6	0	-2.488364	-1.494868	-1.256260
4	6	0	-3.374456	-2.033837	-2.197857
5	6	0	-2.097739	-2.284646	-0.169024
6	6	0	-3.861285	-3.327254	-2.048347
7	1	0	-3.686739	-1.436487	-3.049516
8	6	0	-2.577499	-3.583351	-0.026912
9	1	0	-1.418490	-1.875068	0.570823
10	6	0	-3.465758	-4.107435	-0.962570
11	1	0	-4.550101	-3.728539	-2.785254
12	1	0	-2.261551	-4.180722	0.822982
13	6	0	-0.574518	1.613235	-1.786604
14	6	0	0.440853	2.322150	-2.601938
15	6	0	0.318447	3.705418	-2.786520
16	6	0	1.556618	1.666663	-3.135650
17	6	0	1.290954	4.415132	-3.482840
18	1	0	-0.537849	4.227548	-2.371554
19	6	0	2.538425	2.382497	-3.813985
20	1	0	1.657475	0.592547	-3.014635
21	6	0	2.409886	3.758129	-3.991655
22	1	0	1.180528	5.487019	-3.616597
23	1	0	3.400858	1.858057	-4.215266
24	8	0	-1.916881	1.996834	-2.132821
25	7	0	-2.720606	0.949873	-1.795672
26	6	0	-4.017266	1.184630	-1.836543
27	6	0	-5.007063	0.392787	-1.133527
28	6	0	-4.756209	-0.163569	0.134705
29	6	0	-6.272853	0.215502	-1.717133
30	6	0	-5.719605	-0.923128	0.773938
31	1	0	-3.808673	0.015707	0.628320
32	6	0	-7.243975	-0.542605	-1.085586

33	1	0	-6.482271	0.658102	-2.685483
34	6	0	-6.947398	-1.115255	0.147721
35	1	0	-5.529547	-1.358152	1.746896
36	1	0	-8.213449	-0.701765	-1.540619
37	79	0	0.992418	-0.797241	-0.686155
38	15	0	2.820439	-1.945441	0.200492
39	6	0	2.434683	-3.676880	0.622341
40	6	0	1.411332	-4.322007	-0.081887
41	6	0	3.130231	-4.367956	1.620048
42	6	0	1.092924	-5.646117	0.204276
43	1	0	0.859360	-3.785959	-0.849867
44	6	0	2.807655	-5.692070	1.903423
45	1	0	3.918721	-3.874400	2.180333
46	6	0	1.790411	-6.331035	1.197041
47	1	0	0.294038	-6.137120	-0.342371
48	1	0	3.348725	-6.222868	2.680290
49	1	0	1.537738	-7.361954	1.424664
50	6	0	4.230921	-1.982491	-0.956667
51	6	0	4.560774	-0.787593	-1.610293
52	6	0	4.977441	-3.136137	-1.203127
53	6	0	5.633191	-0.749251	-2.493729
54	1	0	3.979530	0.112719	-1.425608
55	6	0	6.047379	-3.093689	-2.095438
56	1	0	4.728852	-4.067834	-0.704456
57	6	0	6.375808	-1.903944	-2.739234
58	1	0	5.884503	0.180178	-2.995009
59	1	0	6.622831	-3.994033	-2.286327
60	1	0	7.209289	-1.875368	-3.434250
61	6	0	3.466947	-1.188026	1.727516
62	6	0	4.825629	-1.227567	2.055545
63	6	0	2.561848	-0.564029	2.592914
64	6	0	5.269867	-0.653380	3.243489
65	1	0	5.537466	-1.699785	1.384853
66	6	0	3.010142	0.006262	3.779719
67	1	0	1.507562	-0.515420	2.334942
68	6	0	4.363981	-0.038133	4.105037
69	1	0	6.325776	-0.683442	3.493119
70	1	0	2.303979	0.497428	4.440371
71	1	0	4.714977	0.414592	5.027152
72	7	0	-0.147530	2.554819	0.726290
73	16	0	-1.475676	2.698175	1.669632
74	8	0	-1.399702	3.847379	2.549859
75	8	0	-2.622358	2.474966	0.811370
76	16	0	1.333148	3.165468	1.107032
77	8	0	1.635590	3.032070	2.517073
78	8	0	2.236441	2.666904	0.090834
79	7	0	-7.956872	-1.932369	0.808540
80	8	0	-9.037458	-2.078810	0.250962
81	8	0	-7.676159	-2.434926	1.889406
82	1	0	3.174987	4.314595	-4.524192
83	1	0	-3.849763	-5.116177	-0.846990
84	6	0	-1.399189	1.191141	2.750310
85	6	0	1.145877	5.006392	0.779672
86	9	0	-0.399939	1.273249	3.611731
87	9	0	-2.548676	1.095527	3.405295
88	9	0	-1.238903	0.108259	1.992728
89	9	0	1.024148	5.652102	1.926315
90	9	0	0.078509	5.239273	0.027506
91	9	0	2.231416	5.424871	0.146515
92	1	0	-4.305027	2.067576	-2.393047
93	1	0	-0.340300	2.115093	-0.423494

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.777735	-2.411967	0.604678
2	6	0	0.610083	-1.828466	1.152642
3	6	0	2.011609	-2.851193	-0.782721
4	6	0	2.557612	-4.111135	-1.049215
5	6	0	1.646235	-2.014105	-1.839672
6	6	0	2.725972	-4.528276	-2.364487
7	1	0	2.840866	-4.762442	-0.228982
8	6	0	1.828395	-2.431969	-3.154400
9	1	0	1.236124	-1.031926	-1.633788
10	6	0	2.364457	-3.689705	-3.418512
11	1	0	3.141450	-5.510184	-2.567249
12	1	0	1.555088	-1.769934	-3.970053
13	6	0	0.924765	-1.724847	2.491256
14	6	0	0.131868	-1.275356	3.641641
15	6	0	0.725316	-0.518521	4.657941
16	6	0	-1.236660	-1.562467	3.698181
17	6	0	-0.051264	-0.033779	5.704972
18	1	0	1.784913	-0.288509	4.612917
19	6	0	-2.006642	-1.079249	4.750111
20	1	0	-1.691947	-2.167307	2.920114
21	6	0	-1.417041	-0.308678	5.750588
22	1	0	0.410482	0.564999	6.483373
23	1	0	-3.067012	-1.308693	4.788548
24	8	0	2.176291	-2.120446	2.760743
25	7	0	2.718396	-2.574105	1.536424
26	6	0	4.080185	-2.837105	1.483182
27	6	0	4.945056	-1.923608	0.880762
28	6	0	4.521627	-0.661477	0.343997
29	6	0	6.341740	-2.230660	0.756842
30	6	0	5.402674	0.191953	-0.268704
31	1	0	3.483611	-0.357387	0.433474
32	6	0	7.218307	-1.374618	0.144272
33	1	0	6.704743	-3.173392	1.156419
34	6	0	6.761028	-0.151959	-0.383702
35	1	0	5.058573	1.141492	-0.661694
36	1	0	8.268377	-1.628817	0.057300
37	79	0	-1.103966	-1.210564	0.202144
38	15	0	-3.089357	-0.546720	-0.839539
39	6	0	-3.648956	-1.714838	-2.123277
40	6	0	-3.308597	-3.065555	-1.989635
41	6	0	-4.422678	-1.300324	-3.212850
42	6	0	-3.745816	-3.992360	-2.931421
43	1	0	-2.696713	-3.391465	-1.152394
44	6	0	-4.855108	-2.230435	-4.153185
45	1	0	-4.682252	-0.252784	-3.333180
46	6	0	-4.518243	-3.575337	-4.012956
47	1	0	-3.475706	-5.037934	-2.823319
48	1	0	-5.453318	-1.903049	-4.997563
49	1	0	-4.854406	-4.297692	-4.750217
50	6	0	-4.475788	-0.361087	0.331629
51	6	0	-4.189403	-0.190004	1.689706
52	6	0	-5.806672	-0.347929	-0.100431
53	6	0	-5.220277	0.002496	2.605440
54	1	0	-3.159832	-0.212574	2.033599
55	6	0	-6.834224	-0.161608	0.818249
56	1	0	-6.045049	-0.484167	-1.150897
57	6	0	-6.542504	0.016112	2.170194
58	1	0	-4.987053	0.137938	3.656926
59	1	0	-7.864722	-0.154986	0.477859
60	1	0	-7.347664	0.161611	2.883602

61	6	0	-2.957309	1.063499	-1.696500
62	6	0	-3.610175	2.209156	-1.231149
63	6	0	-2.112647	1.152830	-2.812922
64	6	0	-3.421415	3.429648	-1.878267
65	1	0	-4.259884	2.157076	-0.363748
66	6	0	-1.932719	2.372234	-3.456554
67	1	0	-1.589389	0.271618	-3.172378
68	6	0	-2.586332	3.511946	-2.988102
69	1	0	-3.924419	4.315649	-1.505483
70	1	0	-1.269288	2.434426	-4.312847
71	1	0	-2.435533	4.465087	-3.484479
72	7	0	-0.167865	2.399957	-0.265260
73	16	0	1.248726	2.184495	-1.140176
74	8	0	2.355403	2.048999	-0.226735
75	8	0	0.927230	1.198391	-2.144967
76	16	0	-0.345679	3.405499	1.058675
77	8	0	0.764809	4.327737	1.079102
78	8	0	-1.727031	3.820750	1.098329
79	7	0	7.666857	0.730370	-1.022828
80	8	0	8.859758	0.410177	-1.102318
81	8	0	7.240798	1.795966	-1.485934
82	1	0	-2.020007	0.073546	6.568308
83	1	0	2.503477	-4.017092	-4.444195
84	6	0	1.458063	3.824394	-2.043340
85	6	0	-0.105394	2.206604	2.458629
86	9	0	2.377937	4.541501	-1.434178
87	9	0	1.835250	3.546385	-3.277722
88	9	0	0.306365	4.476562	-2.059888
89	9	0	-0.054806	2.896656	3.584211
90	9	0	1.017467	1.536693	2.281648
91	9	0	-1.137854	1.379744	2.480418
92	1	0	4.411826	-3.761412	1.937952
93	1	0	-1.030632	2.086205	-0.722139

Ts3d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.447425	0.912241	1.227760
2	6	0	-0.534735	-0.189837	1.162639
3	6	0	-1.465733	2.085977	0.338799
4	6	0	-1.625130	3.378969	0.845601
5	6	0	-1.260349	1.892406	-1.031431
6	6	0	-1.571148	4.468527	-0.016270
7	1	0	-1.789197	3.528344	1.907548
8	6	0	-1.222803	2.985444	-1.889547
9	1	0	-1.134134	0.890144	-1.425333
10	6	0	-1.376566	4.273912	-1.383274
11	1	0	-1.686114	5.472074	0.380327
12	1	0	-1.069242	2.828432	-2.952097
13	6	0	-0.883915	-0.935892	2.284766
14	6	0	-0.352360	-2.188443	2.820978
15	6	0	-1.201788	-3.051275	3.527980
16	6	0	0.981098	-2.554332	2.599603
17	6	0	-0.719107	-4.264885	4.000515
18	1	0	-2.239973	-2.779739	3.684355
19	6	0	1.455721	-3.771075	3.072983
20	1	0	1.646949	-1.879468	2.070289
21	6	0	0.607476	-4.627343	3.772356
22	1	0	-1.382165	-4.933079	4.540028
23	1	0	2.490905	-4.047482	2.900758

24	8	0	-1.935762	-0.434944	2.922061
25	7	0	-2.295423	0.777829	2.234953
26	6	0	-3.433124	1.425538	2.657252
27	6	0	-4.538908	1.590180	1.810964
28	6	0	-4.620697	1.061914	0.485993
29	6	0	-5.663034	2.350407	2.265268
30	6	0	-5.717503	1.277906	-0.311228
31	1	0	-3.805243	0.465571	0.097224
32	6	0	-6.757406	2.568708	1.467250
33	1	0	-5.641260	2.765844	3.268579
34	6	0	-6.794630	2.038587	0.166305
35	1	0	-5.759406	0.859857	-1.309698
36	1	0	-7.597661	3.150023	1.828465
37	79	0	1.415688	0.241888	0.492733
38	15	0	3.515983	1.035041	-0.085244
39	6	0	3.403655	2.553535	-1.088430
40	6	0	2.350317	3.442202	-0.842115
41	6	0	4.352845	2.857572	-2.069090
42	6	0	2.256946	4.628771	-1.561915
43	1	0	1.598315	3.204686	-0.093220
44	6	0	4.249809	4.043246	-2.791697
45	1	0	5.170694	2.172677	-2.271428
46	6	0	3.205268	4.929241	-2.537407
47	1	0	1.435955	5.310918	-1.366719
48	1	0	4.986641	4.272864	-3.554778
49	1	0	3.127116	5.851880	-3.103996
50	6	0	4.512516	1.466755	1.380027
51	6	0	4.454865	0.619926	2.493708
52	6	0	5.341721	2.591036	1.407359
53	6	0	5.224759	0.893048	3.619182
54	1	0	3.806001	-0.252415	2.481307
55	6	0	6.105673	2.864104	2.539635
56	1	0	5.392996	3.255503	0.550486
57	6	0	6.049365	2.016681	3.643250
58	1	0	5.175521	0.232861	4.479246
59	1	0	6.744992	3.741012	2.557055
60	1	0	6.644525	2.233876	4.524725
61	6	0	4.537861	-0.125704	-1.051722
62	6	0	5.902875	-0.295076	-0.805275
63	6	0	3.922223	-0.842828	-2.084545
64	6	0	6.645093	-1.176313	-1.588373
65	1	0	6.389432	0.255887	-0.006451
66	6	0	4.669994	-1.716213	-2.866654
67	1	0	2.859953	-0.718352	-2.275735
68	6	0	6.031176	-1.884900	-2.617972
69	1	0	7.704517	-1.307257	-1.391851
70	1	0	4.187144	-2.270342	-3.664778
71	1	0	6.612464	-2.571675	-3.225387
72	7	0	-1.164790	-1.847335	-0.825718
73	16	0	-2.589121	-2.642726	-0.520421
74	8	0	-2.499496	-4.060092	-0.789242
75	8	0	-3.030641	-2.136311	0.763220
76	16	0	-0.242622	-2.122096	-2.159889
77	8	0	-1.021667	-2.783852	-3.184729
78	8	0	0.494354	-0.905918	-2.439525
79	7	0	-7.925712	2.270396	-0.665626
80	8	0	-8.864858	2.938425	-0.221394
81	8	0	-7.933280	1.796983	-1.806350
82	1	0	0.980323	-5.577896	4.140614
83	1	0	-1.343810	5.127452	-2.053082
84	6	0	-3.783855	-1.930275	-1.780431
85	6	0	1.014992	-3.356623	-1.571378
86	9	0	-3.835943	-2.695281	-2.852231
87	9	0	-4.975045	-1.885469	-1.205642
88	9	0	-3.405640	-0.703299	-2.120370

89	9	0	1.855629	-3.583021	-2.570800
90	9	0	0.414729	-4.479509	-1.221796
91	9	0	1.682050	-2.868650	-0.532718
92	1	0	-3.416605	1.786800	3.677335
93	1	0	-0.786785	-1.085010	0.009798

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.144606	-1.870937	0.020412
2	6	0	0.777602	-0.791845	0.879738
3	6	0	0.993787	-1.807180	-1.461527
4	6	0	1.017607	-2.991386	-2.211736
5	6	0	0.777471	-0.588012	-2.117763
6	6	0	0.830076	-2.954270	-3.588244
7	1	0	1.156433	-3.947614	-1.720127
8	6	0	0.592004	-0.557281	-3.492825
9	1	0	0.763453	0.345820	-1.571229
10	6	0	0.612871	-1.738268	-4.232102
11	1	0	0.842596	-3.879017	-4.155810
12	1	0	0.427369	0.397145	-3.981766
13	6	0	1.041159	-0.866582	2.341318
14	6	0	0.782198	0.349453	3.188147
15	6	0	0.919164	0.204033	4.573246
16	6	0	0.409070	1.592794	2.668190
17	6	0	0.683051	1.276653	5.423894
18	1	0	1.212431	-0.762794	4.967731
19	6	0	0.173584	2.667656	3.520514
20	1	0	0.313052	1.740607	1.600310
21	6	0	0.308260	2.512264	4.897784
22	1	0	0.791812	1.150815	6.496687
23	1	0	-0.109989	3.628543	3.105786
24	8	0	1.408013	-1.902015	2.885457
25	7	0	1.516719	-3.054183	0.495587
26	6	0	2.594601	-3.673015	0.727685
27	6	0	3.957913	-3.126523	0.603701
28	6	0	4.210130	-1.772068	0.354205
29	6	0	5.025199	-4.019352	0.755258
30	6	0	5.513577	-1.314566	0.240597
31	1	0	3.407449	-1.050666	0.259383
32	6	0	6.334598	-3.575335	0.642910
33	1	0	4.827079	-5.066603	0.960604
34	6	0	6.550649	-2.227972	0.384246
35	1	0	5.721327	-0.270622	0.046172
36	1	0	7.170296	-4.254338	0.752955
37	79	0	-1.404611	-0.798133	0.569077
38	15	0	-3.626304	-0.783273	-0.058213
39	6	0	-3.826302	-1.554330	-1.697902
40	6	0	-2.872885	-2.477026	-2.141359
41	6	0	-4.912744	-1.231114	-2.518240
42	6	0	-3.010582	-3.078523	-3.388470
43	1	0	-2.014402	-2.714045	-1.517730
44	6	0	-5.046672	-1.836401	-3.764019
45	1	0	-5.649828	-0.504706	-2.188787
46	6	0	-4.097232	-2.759289	-4.199156
47	1	0	-2.261910	-3.786401	-3.729174
48	1	0	-5.890268	-1.581604	-4.397509
49	1	0	-4.201336	-3.223695	-5.174826
50	6	0	-4.722595	-1.664270	1.098970
51	6	0	-4.478319	-1.520653	2.470332

52	6	0	-5.800540	-2.439528	0.663451
53	6	0	-5.312281	-2.138571	3.395709
54	1	0	-3.635018	-0.926052	2.812896
55	6	0	-6.628137	-3.062099	1.594772
56	1	0	-5.996843	-2.563040	-0.396907
57	6	0	-6.387107	-2.910584	2.958006
58	1	0	-5.118198	-2.022769	4.457219
59	1	0	-7.462069	-3.666417	1.252244
60	1	0	-7.034286	-3.397900	3.680550
61	6	0	-4.312391	0.895780	-0.237171
62	6	0	-5.570021	1.246291	0.259105
63	6	0	-3.540844	1.843822	-0.919145
64	6	0	-6.051215	2.540556	0.071774
65	1	0	-6.174783	0.517668	0.790045
66	6	0	-4.028902	3.131597	-1.106700
67	1	0	-2.555979	1.585517	-1.299938
68	6	0	-5.283497	3.481503	-0.609744
69	1	0	-7.027529	2.811639	0.460996
70	1	0	-3.419901	3.863067	-1.627083
71	1	0	-5.660520	4.489838	-0.750008
72	7	0	1.406002	2.251791	-0.588539
73	16	0	2.936791	2.453533	-0.145536
74	8	0	3.364719	3.828353	0.059833
75	8	0	3.226777	1.455258	0.876070
76	16	0	0.535393	3.312315	-1.419434
77	8	0	1.277119	4.353769	-2.114165
78	8	0	-0.490851	2.571524	-2.145424
79	7	0	7.932319	-1.747766	0.261142
80	8	0	8.834969	-2.555789	0.421901
81	8	0	8.105701	-0.566559	0.003192
82	1	0	0.124259	3.352982	5.559808
83	1	0	0.456986	-1.711386	-5.305924
84	6	0	3.888633	1.858963	-1.619418
85	6	0	-0.398093	4.197107	-0.089481
86	9	0	3.561198	2.543286	-2.708766
87	9	0	5.190417	2.012595	-1.382706
88	9	0	3.643778	0.566977	-1.834212
89	9	0	-1.145781	5.150481	-0.639374
90	9	0	0.443084	4.750026	0.777970
91	9	0	-1.195922	3.351892	0.563420
92	1	0	2.514151	-4.707909	1.059826
93	1	0	0.875526	0.190499	0.416287

TS4d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.126569	-1.512144	1.359798
2	6	0	-0.858821	-0.950378	0.026640
3	6	0	-0.532056	-0.918126	2.585705
4	6	0	-0.369052	-1.721979	3.719751
5	6	0	-0.096037	0.411048	2.615135
6	6	0	0.231183	-1.205965	4.862817
7	1	0	-0.696690	-2.756664	3.695104
8	6	0	0.498231	0.924173	3.761409
9	1	0	-0.227945	1.056948	1.756292
10	6	0	0.669354	0.117183	4.884313
11	1	0	0.363879	-1.839462	5.734079
12	1	0	0.829316	1.957420	3.769670
13	6	0	-1.364787	-1.635352	-1.172304
14	6	0	-1.365205	-0.920085	-2.491324

15	6	0	-1.805509	-1.627332	-3.615341
16	6	0	-0.950665	0.407762	-2.640349
17	6	0	-1.825748	-1.022193	-4.866427
18	1	0	-2.132020	-2.654188	-3.493847
19	6	0	-0.973259	1.013143	-3.891830
20	1	0	-0.622197	0.983263	-1.784716
21	6	0	-1.407919	0.299921	-5.007077
22	1	0	-2.169152	-1.580705	-5.731618
23	1	0	-0.655319	2.045144	-3.992624
24	8	0	-1.745908	-2.819852	-1.166785
25	7	0	-1.849339	-2.564267	1.512268
26	6	0	-2.617275	-3.316562	0.797888
27	6	0	-4.010940	-2.954673	0.515757
28	6	0	-4.465353	-1.648308	0.730706
29	6	0	-4.857938	-3.921557	-0.034739
30	6	0	-5.763175	-1.302534	0.392600
31	1	0	-3.808543	-0.896601	1.150732
32	6	0	-6.163320	-3.589665	-0.367594
33	1	0	-4.493559	-4.929391	-0.205062
34	6	0	-6.586302	-2.285002	-0.145886
35	1	0	-6.127384	-0.294129	0.539815
36	1	0	-6.839760	-4.320329	-0.791811
37	79	0	1.297327	-0.913992	-0.177624
38	15	0	3.608225	-0.767500	-0.128916
39	6	0	4.220513	-0.752665	1.589337
40	6	0	3.460065	-1.369682	2.588861
41	6	0	5.434034	-0.140343	1.921129
42	6	0	3.915658	-1.384721	3.903650
43	1	0	2.504870	-1.827088	2.342442
44	6	0	5.884023	-0.156055	3.237908
45	1	0	6.025539	0.352480	1.155227
46	6	0	5.126813	-0.778523	4.228521
47	1	0	3.316073	-1.858815	4.673955
48	1	0	6.824618	0.323137	3.490275
49	1	0	5.477970	-0.783900	5.255700
50	6	0	4.450363	-2.141743	-0.979720
51	6	0	3.910298	-2.590995	-2.191154
52	6	0	5.612865	-2.732141	-0.477522
53	6	0	4.534663	-3.614065	-2.896403
54	1	0	3.000914	-2.139936	-2.580857
55	6	0	6.229941	-3.761741	-1.184284
56	1	0	6.038877	-2.395179	0.462172
57	6	0	5.694171	-4.201141	-2.392167
58	1	0	4.111878	-3.957322	-3.835202
59	1	0	7.130644	-4.219861	-0.788172
60	1	0	6.177448	-5.004498	-2.939406
61	6	0	4.255530	0.763072	-0.878298
62	6	0	5.383604	0.774675	-1.702277
63	6	0	3.593497	1.960509	-0.583742
64	6	0	5.845327	1.980200	-2.226605
65	1	0	5.902519	-0.149485	-1.937575
66	6	0	4.061753	3.160468	-1.106786
67	1	0	2.710091	1.961479	0.049629
68	6	0	5.186642	3.170971	-1.929920
69	1	0	6.720409	1.986124	-2.868823
70	1	0	3.536400	4.082624	-0.881758
71	1	0	5.547454	4.107616	-2.343526
72	7	0	-1.348029	2.386970	0.144221
73	16	0	-2.944545	2.471835	-0.009574
74	8	0	-3.476695	3.741709	-0.479724
75	8	0	-3.395865	1.235562	-0.632756
76	16	0	-0.365525	3.638942	0.326811
77	8	0	-0.973858	4.879415	0.782667
78	8	0	0.843493	3.163282	0.991079
79	7	0	-7.967960	-1.926981	-0.497344

80	8	0	-8.678629	-2.796844	-0.977624
81	8	0	-8.330557	-0.779992	-0.287997
82	1	0	-1.424236	0.775082	-5.983232
83	1	0	1.145415	0.517392	5.774039
84	6	0	-3.523540	2.312469	1.739914
85	6	0	0.178742	3.973230	-1.410031
86	9	0	-3.065137	3.310371	2.485602
87	9	0	-4.854757	2.322982	1.761406
88	9	0	-3.100512	1.158943	2.262259
89	9	0	0.964129	5.047607	-1.426265
90	9	0	-0.871584	4.189216	-2.194776
91	9	0	0.865913	2.935691	-1.888865
92	1	0	-2.310577	-4.345202	0.620550
93	1	0	-1.011867	0.130985	0.019339

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.129919	-1.416555	1.560064
2	6	0	-0.989227	-0.778610	0.227567
3	6	0	-0.512189	-0.768095	2.750387
4	6	0	-0.303381	-1.523075	3.910874
5	6	0	-0.098494	0.569019	2.723697
6	6	0	0.315008	-0.954460	5.017685
7	1	0	-0.621440	-2.559873	3.930333
8	6	0	0.521396	1.135095	3.833308
9	1	0	-0.258230	1.185875	1.847458
10	6	0	0.734662	0.375438	4.979977
11	1	0	0.477927	-1.551695	5.909548
12	1	0	0.837615	2.172441	3.793019
13	6	0	-1.354198	-1.552659	-0.878916
14	6	0	-1.406660	-1.101010	-2.278307
15	6	0	-1.876577	-1.975071	-3.266163
16	6	0	-1.029433	0.202565	-2.628878
17	6	0	-1.950079	-1.552444	-4.588697
18	1	0	-2.190245	-2.976694	-2.996356
19	6	0	-1.111507	0.620714	-3.947782
20	1	0	-0.681151	0.892849	-1.871262
21	6	0	-1.567064	-0.257897	-4.931415
22	1	0	-2.313874	-2.233633	-5.350861
23	1	0	-0.822682	1.633878	-4.205269
24	8	0	-1.685042	-2.818486	-0.706151
25	7	0	-1.725175	-2.543336	1.718236
26	6	0	-2.315714	-3.164993	0.584091
27	6	0	-3.796213	-2.856865	0.432879
28	6	0	-4.321904	-1.621934	0.815159
29	6	0	-4.617724	-3.801776	-0.185620
30	6	0	-5.654906	-1.320384	0.571478
31	1	0	-3.701063	-0.879824	1.300685
32	6	0	-5.955271	-3.521348	-0.427043
33	1	0	-4.208729	-4.762299	-0.483580
34	6	0	-6.448049	-2.279231	-0.044752
35	1	0	-6.066787	-0.358900	0.850716
36	1	0	-6.605476	-4.245346	-0.901435
37	79	0	1.206007	-0.811365	-0.137101
38	15	0	3.513714	-0.771013	-0.118167
39	6	0	4.136021	-0.773659	1.594212
40	6	0	3.372573	-1.380816	2.597447
41	6	0	5.365153	-0.187912	1.914965
42	6	0	3.840583	-1.411042	3.907195
43	1	0	2.406357	-1.818156	2.358541

44	6	0	5.826929	-0.218575	3.227525
45	1	0	5.959225	0.294992	1.144849
46	6	0	5.066750	-0.829986	4.222490
47	1	0	3.239425	-1.876966	4.681027
48	1	0	6.779432	0.240189	3.472872
49	1	0	5.427334	-0.846752	5.246238
50	6	0	4.256770	-2.202516	-0.963292
51	6	0	3.663635	-2.650970	-2.149741
52	6	0	5.406192	-2.832634	-0.479213
53	6	0	4.222195	-3.715452	-2.848654
54	1	0	2.765044	-2.167343	-2.525331
55	6	0	5.956925	-3.902956	-1.179900
56	1	0	5.872884	-2.495101	0.440762
57	6	0	5.368198	-4.342960	-2.362747
58	1	0	3.758760	-4.058996	-3.767901
59	1	0	6.847356	-4.392493	-0.798596
60	1	0	5.800172	-5.178323	-2.904859
61	6	0	4.228541	0.712509	-0.894618
62	6	0	5.310545	0.644988	-1.775341
63	6	0	3.671530	1.952588	-0.562731
64	6	0	5.830776	1.816858	-2.320824
65	1	0	5.747796	-0.313408	-2.037573
66	6	0	4.197679	3.117764	-1.108062
67	1	0	2.822475	2.012988	0.112809
68	6	0	5.276465	3.050499	-1.988560
69	1	0	6.670120	1.762976	-3.006930
70	1	0	3.753472	4.074630	-0.854753
71	1	0	5.682752	3.960523	-2.419037
72	7	0	-1.317455	2.443645	-0.003080
73	16	0	-2.908785	2.600744	-0.164829
74	8	0	-3.381309	3.882965	-0.663001
75	8	0	-3.415696	1.373333	-0.761005
76	16	0	-0.261923	3.644007	0.087618
77	8	0	-0.796781	4.958869	0.404676
78	8	0	0.902102	3.163751	0.824332
79	7	0	-7.857180	-1.970488	-0.302346
80	8	0	-8.536988	-2.818059	-0.863421
81	8	0	-8.281080	-0.881766	0.056568
82	1	0	-1.628306	0.070169	-5.964345
83	1	0	1.226097	0.815902	5.841973
84	6	0	-3.477419	2.508993	1.592214
85	6	0	0.325633	3.765009	-1.664034
86	9	0	-2.961907	3.505292	2.303820
87	9	0	-4.805423	2.583568	1.628623
88	9	0	-3.100366	1.352329	2.139248
89	9	0	1.170975	4.784926	-1.779123
90	9	0	-0.702791	3.955003	-2.485313
91	9	0	0.955558	2.644881	-2.023078
92	1	0	-2.157682	-4.242454	0.634506
93	1	0	-1.084289	0.303325	0.150811

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.231333	1.898357	0.822291
2	6	0	-0.717382	0.506610	0.838418
3	6	0	-0.584069	2.894075	-0.082740
4	6	0	-0.334120	4.190086	0.377212
5	6	0	-0.218989	2.552705	-1.389869
6	6	0	0.282633	5.124786	-0.450123
7	1	0	-0.619541	4.456036	1.390075

8	6	0	0.382850	3.491992	-2.221154
9	1	0	-0.410272	1.555444	-1.767131
10	6	0	0.640490	4.778461	-1.751913
11	1	0	0.482695	6.124914	-0.077734
12	1	0	0.654871	3.214576	-3.234834
13	6	0	-1.256429	-0.256462	1.851457
14	6	0	-0.856800	-1.655685	2.156887
15	6	0	-1.789264	-2.683080	1.984653
16	6	0	0.431227	-1.958380	2.607824
17	6	0	-1.415558	-4.004886	2.207375
18	1	0	-2.793035	-2.444165	1.650923
19	6	0	0.793806	-3.280209	2.849073
20	1	0	1.142559	-1.157454	2.783370
21	6	0	-0.124084	-4.306025	2.635654
22	1	0	-2.136546	-4.800460	2.047949
23	1	0	1.793970	-3.507304	3.205402
24	8	0	-2.217518	0.150884	2.670517
25	7	0	-2.169125	2.343490	1.579223
26	6	0	-2.847928	1.452210	2.459355
27	6	0	-4.286400	1.200602	2.027873
28	6	0	-4.879545	1.965542	1.025681
29	6	0	-5.017754	0.189299	2.656051
30	6	0	-6.184000	1.708043	0.624412
31	1	0	-4.313184	2.753834	0.545504
32	6	0	-6.321163	-0.079701	2.269178
33	1	0	-4.558974	-0.407993	3.436391
34	6	0	-6.882018	0.684543	1.251230
35	1	0	-6.650272	2.283431	-0.165194
36	1	0	-6.895312	-0.867765	2.739738
37	79	0	1.346749	0.285495	0.424561
38	15	0	3.662738	0.242817	0.230773
39	6	0	4.351463	1.785513	-0.455362
40	6	0	3.591283	2.957832	-0.381424
41	6	0	5.631754	1.824498	-1.018614
42	6	0	4.112018	4.158127	-0.857073
43	1	0	2.589725	2.933019	0.041475
44	6	0	6.145253	3.025426	-1.497485
45	1	0	6.227994	0.919386	-1.085999
46	6	0	5.387125	4.192475	-1.415228
47	1	0	3.513941	5.061771	-0.799009
48	1	0	7.137712	3.049424	-1.936246
49	1	0	5.789756	5.127754	-1.791655
50	6	0	4.421409	0.045145	1.881862
51	6	0	4.084109	-1.098252	2.618753
52	6	0	5.276490	0.997150	2.438164
53	6	0	4.602022	-1.286505	3.894233
54	1	0	3.417087	-1.842626	2.190583
55	6	0	5.787965	0.807520	3.721680
56	1	0	5.546455	1.887266	1.878769
57	6	0	5.453370	-0.330463	4.448978
58	1	0	4.338791	-2.176096	4.457880
59	1	0	6.450967	1.552911	4.149564
60	1	0	5.853409	-0.474037	5.447851
61	6	0	4.367006	-1.109597	-0.771592
62	6	0	5.563901	-1.745242	-0.426287
63	6	0	3.687255	-1.494266	-1.931963
64	6	0	6.072704	-2.756624	-1.236876
65	1	0	6.098866	-1.457143	0.473408
66	6	0	4.201296	-2.503778	-2.739645
67	1	0	2.753490	-1.009242	-2.199596
68	6	0	5.392778	-3.136803	-2.391952
69	1	0	7.000639	-3.248903	-0.963234
70	1	0	3.664125	-2.800732	-3.634678
71	1	0	5.789898	-3.929130	-3.018949
72	7	0	-1.535133	-0.870634	-1.384851

73	16	0	-3.173870	-1.082210	-1.362283
74	8	0	-3.604544	-2.234901	-2.120245
75	8	0	-3.591547	-0.885266	0.009152
76	16	0	-0.543392	-1.442168	-2.570695
77	8	0	-1.270446	-1.833306	-3.757916
78	8	0	0.587709	-0.539789	-2.660400
79	7	0	-8.252017	0.399892	0.826862
80	8	0	-8.850158	-0.511069	1.383132
81	8	0	-8.734194	1.086046	-0.064010
82	1	0	0.162904	-5.338047	2.812313
83	1	0	1.120418	5.507505	-2.397619
84	6	0	-3.746345	0.424055	-2.278616
85	6	0	0.091641	-3.011258	-1.807037
86	9	0	-3.296243	0.395489	-3.523928
87	9	0	-5.071304	0.437068	-2.278694
88	9	0	-3.288225	1.509206	-1.669506
89	9	0	0.891056	-3.601507	-2.684611
90	9	0	-0.927643	-3.805038	-1.519049
91	9	0	0.770307	-2.745623	-0.699163
92	1	0	-2.857293	1.891195	3.463009
93	1	0	-1.067943	-0.287089	-0.432571

2d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.722991	1.096743	0.389171
2	6	0	-2.274601	-0.243942	0.503499
3	6	0	-2.621362	2.257152	0.144009
4	6	0	-2.175136	3.548388	0.449882
5	6	0	-3.900653	2.090905	-0.396473
6	6	0	-2.992269	4.648662	0.223665
7	1	0	-1.183895	3.674830	0.871917
8	6	0	-4.716700	3.194721	-0.627240
9	1	0	-4.258529	1.100873	-0.660035
10	6	0	-4.266113	4.474527	-0.315895
11	1	0	-2.637444	5.644191	0.471421
12	1	0	-5.704421	3.053384	-1.054490
13	6	0	-1.438338	-1.273405	0.225469
14	6	0	-1.821280	-2.675829	-0.013148
15	6	0	-3.126517	-3.011114	-0.394341
16	6	0	-0.870164	-3.690837	0.144743
17	6	0	-3.476354	-4.340713	-0.594368
18	1	0	-3.864023	-2.231530	-0.554884
19	6	0	-1.223448	-5.019460	-0.062249
20	1	0	0.142078	-3.433394	0.435802
21	6	0	-2.526632	-5.347410	-0.428324
22	1	0	-4.489412	-4.591220	-0.892080
23	1	0	-0.480494	-5.800090	0.065948
24	8	0	-0.116986	-1.042439	0.094936
25	7	0	-0.448868	1.307689	0.438336
26	6	0	0.316374	0.148096	0.794930
27	1	0	0.184165	-0.061656	1.870637
28	6	0	1.787768	0.289392	0.480042
29	6	0	2.254073	1.296780	-0.362000
30	6	0	2.683897	-0.632201	1.026865
31	6	0	3.606929	1.388764	-0.663485
32	1	0	1.552353	2.012854	-0.773206
33	6	0	4.037622	-0.556938	0.736158
34	1	0	2.320363	-1.413285	1.687456
35	6	0	4.474772	0.457440	-0.108545
36	1	0	3.984534	2.165525	-1.316223

37	1	0	4.744128	-1.262648	1.154063
38	7	0	5.902535	0.548869	-0.419832
39	8	0	6.655184	-0.276119	0.079937
40	8	0	6.274210	1.444989	-1.164937
41	1	0	-2.801354	-6.385096	-0.589595
42	1	0	-4.904721	5.334406	-0.492783
43	1	0	-3.331537	-0.412826	0.652855

TS5d'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.952755	1.120901	1.007840
2	6	0	1.769542	-0.244260	0.469981
3	6	0	1.158349	1.577960	2.182123
4	6	0	0.871906	2.943436	2.310481
5	6	0	0.669406	0.682459	3.138449
6	6	0	0.116123	3.404584	3.380601
7	1	0	1.233362	3.631673	1.553560
8	6	0	-0.074942	1.151156	4.218509
9	1	0	0.864588	-0.381623	3.052035
10	6	0	-0.354821	2.509391	4.341409
11	1	0	-0.113040	4.462691	3.460099
12	1	0	-0.446018	0.448337	4.956503
13	6	0	2.299218	-0.493605	-0.780611
14	6	0	2.322596	-1.788482	-1.483175
15	6	0	3.322519	-2.019751	-2.436319
16	6	0	1.397530	-2.798108	-1.192710
17	6	0	3.400174	-3.250099	-3.078720
18	1	0	4.045564	-1.242494	-2.655956
19	6	0	1.479070	-4.024175	-1.838833
20	1	0	0.604961	-2.615126	-0.475742
21	6	0	2.480213	-4.253083	-2.781636
22	1	0	4.182141	-3.425951	-3.810317
23	1	0	0.751379	-4.796255	-1.615716
24	8	0	2.881963	0.489282	-1.465739
25	7	0	2.742734	1.972457	0.457948
26	6	0	3.496775	1.558626	-0.677125
27	6	0	4.907696	1.104818	-0.329891
28	6	0	5.297581	0.828723	0.979307
29	6	0	5.812921	0.919958	-1.379799
30	6	0	6.579559	0.360372	1.244832
31	1	0	4.607400	0.984913	1.800250
32	6	0	7.093991	0.451715	-1.133105
33	1	0	5.511650	1.141984	-2.398993
34	6	0	7.453358	0.177775	0.182337
35	1	0	6.895848	0.139641	2.256462
36	1	0	7.803763	0.304166	-1.936982
37	79	0	-0.472614	0.068354	-0.307985
38	15	0	-1.896710	1.791308	-0.874479
39	6	0	-3.261932	1.956228	0.318709
40	6	0	-2.925083	1.964878	1.677741
41	6	0	-4.599259	2.051017	-0.065927
42	6	0	-3.918407	2.079369	2.641870
43	1	0	-1.885132	1.882689	1.983205
44	6	0	-5.592926	2.156686	0.905750
45	1	0	-4.873088	2.034287	-1.115844
46	6	0	-5.255286	2.172782	2.256126
47	1	0	-3.647383	2.084845	3.692982
48	1	0	-6.633114	2.223784	0.603080
49	1	0	-6.033249	2.253638	3.008986

50	6	0	-0.988259	3.376802	-0.783741
51	6	0	0.279344	3.442348	-1.373501
52	6	0	-1.509839	4.502500	-0.142395
53	6	0	1.015173	4.620484	-1.323391
54	1	0	0.696426	2.563807	-1.859787
55	6	0	-0.764289	5.678297	-0.083660
56	1	0	-2.490591	4.465005	0.320672
57	6	0	0.496518	5.738658	-0.671296
58	1	0	1.999219	4.661823	-1.779613
59	1	0	-1.172078	6.547164	0.423273
60	1	0	1.076541	6.654816	-0.620457
61	6	0	-2.613915	1.756132	-2.546626
62	6	0	-3.130858	2.922331	-3.123734
63	6	0	-2.644709	0.555081	-3.260164
64	6	0	-3.681230	2.880165	-4.400295
65	1	0	-3.102166	3.861366	-2.578339
66	6	0	-3.194758	0.518828	-4.538520
67	1	0	-2.249996	-0.350254	-2.812195
68	6	0	-3.712840	1.679101	-5.107852
69	1	0	-4.081936	3.785827	-4.844333
70	1	0	-3.215733	-0.416622	-5.088563
71	1	0	-4.139147	1.649889	-6.105837
72	7	0	-1.599157	-2.139973	0.607655
73	16	0	-1.095199	-2.940796	1.919259
74	8	0	-1.468822	-4.343318	1.993053
75	8	0	0.304455	-2.582914	2.122840
76	16	0	-3.010770	-2.475469	-0.113051
77	8	0	-3.918058	-3.294676	0.675396
78	8	0	-3.516745	-1.268674	-0.747044
79	7	0	8.804455	-0.318011	0.455745
80	8	0	9.557511	-0.484944	-0.493141
81	8	0	9.110497	-0.540571	1.618226
82	1	0	2.539808	-5.211882	-3.287087
83	1	0	-0.944649	2.869502	5.178783
84	6	0	-1.994232	-2.102874	3.321339
85	6	0	-2.464840	-3.532613	-1.530207
86	9	0	-2.193837	-0.818285	3.042280
87	9	0	-3.164963	-2.683845	3.535753
88	9	0	-1.250508	-2.196872	4.420779
89	9	0	-3.529143	-3.903293	-2.233707
90	9	0	-1.832194	-4.614054	-1.089469
91	9	0	-1.643322	-2.843817	-2.324452
92	1	0	3.543762	2.381092	-1.393828
93	1	0	1.497323	-1.074437	1.114508

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.482021	1.170389	0.776475
2	6	0	2.034212	0.042289	-0.019984
3	6	0	1.842186	1.444675	2.092594
4	6	0	1.839623	2.747987	2.603969
5	6	0	1.288895	0.412313	2.857375
6	6	0	1.301601	3.012241	3.857245
7	1	0	2.266682	3.546227	2.006958
8	6	0	0.766825	0.676774	4.122269
9	1	0	1.287623	-0.608172	2.489048
10	6	0	0.771982	1.974651	4.624743
11	1	0	1.297537	4.028497	4.239024
12	1	0	0.359536	-0.136563	4.713110

13	6	0	2.346416	0.055165	-1.336273
14	6	0	1.748664	-0.799294	-2.378822
15	6	0	1.871839	-0.438219	-3.725669
16	6	0	1.038019	-1.958711	-2.042108
17	6	0	1.275869	-1.211751	-4.716982
18	1	0	2.429782	0.452237	-3.992336
19	6	0	0.460020	-2.736560	-3.037909
20	1	0	0.951843	-2.267266	-1.005592
21	6	0	0.569020	-2.362080	-4.376411
22	1	0	1.369974	-0.917068	-5.757449
23	1	0	-0.078083	-3.637638	-2.767442
24	8	0	3.197786	0.973818	-1.825743
25	7	0	3.385444	1.992419	0.359201
26	6	0	4.045821	1.617982	-0.862233
27	6	0	5.268197	0.740175	-0.588457
28	6	0	6.007843	0.925020	0.582399
29	6	0	5.678348	-0.214314	-1.521561
30	6	0	7.141548	0.162982	0.827786
31	1	0	5.686664	1.661801	1.309821
32	6	0	6.806252	-0.989315	-1.288149
33	1	0	5.108660	-0.363324	-2.431807
34	6	0	7.521120	-0.785587	-0.114409
35	1	0	7.720390	0.294302	1.733451
36	1	0	7.127421	-1.739373	-1.999846
37	79	0	-1.526602	-0.198007	0.069374
38	15	0	-1.713703	2.031955	-0.412916
39	6	0	-2.329840	2.948000	1.037444
40	6	0	-1.914639	2.552933	2.313060
41	6	0	-3.179858	4.049266	0.893608
42	6	0	-2.347097	3.254377	3.434362
43	1	0	-1.249207	1.702032	2.432623
44	6	0	-3.611612	4.744578	2.018777
45	1	0	-3.511037	4.364072	-0.090960
46	6	0	-3.197133	4.347709	3.288625
47	1	0	-2.019412	2.941596	4.420365
48	1	0	-4.275505	5.595252	1.902474
49	1	0	-3.539112	4.889825	4.164785
50	6	0	-0.243350	2.936667	-0.989919
51	6	0	0.340506	2.552320	-2.202025
52	6	0	0.272967	4.022779	-0.280950
53	6	0	1.418821	3.266345	-2.709068
54	1	0	-0.051042	1.700481	-2.752282
55	6	0	1.363371	4.725926	-0.788464
56	1	0	-0.171362	4.325327	0.661488
57	6	0	1.930256	4.355165	-2.003998
58	1	0	1.865201	2.967533	-3.651502
59	1	0	1.763944	5.567745	-0.232722
60	1	0	2.774245	4.910361	-2.401453
61	6	0	-2.959807	2.270111	-1.725465
62	6	0	-2.914863	3.373251	-2.584452
63	6	0	-4.005018	1.346155	-1.837440
64	6	0	-3.907011	3.546935	-3.545373
65	1	0	-2.109046	4.096635	-2.508516
66	6	0	-4.995008	1.526801	-2.798173
67	1	0	-4.043820	0.482121	-1.178946
68	6	0	-4.946043	2.625289	-3.653472
69	1	0	-3.865635	4.403451	-4.210719
70	1	0	-5.800166	0.803715	-2.881381
71	1	0	-5.715693	2.761680	-4.406802
72	7	0	-1.874801	-2.283393	0.553602
73	16	0	-0.839627	-3.129348	1.507584
74	8	0	-0.999549	-4.565605	1.419224
75	8	0	0.476170	-2.533806	1.338021
76	16	0	-3.366940	-2.860282	0.151358
77	8	0	-3.794104	-3.970777	0.977900

78	8	0	-4.246571	-1.724025	-0.058432
79	7	0	8.711557	-1.596763	0.138137
80	8	0	9.029625	-2.429411	-0.699810
81	8	0	9.331760	-1.402108	1.174435
82	1	0	0.110812	-2.970127	-5.150224
83	1	0	0.362986	2.179119	5.609522
84	6	0	-1.359550	-2.632830	3.225327
85	6	0	-3.054463	-3.546421	-1.541330
86	9	0	-1.582095	-1.321991	3.273681
87	9	0	-2.462515	-3.273596	3.574044
88	9	0	-0.377620	-2.939094	4.063205
89	9	0	-2.680110	-2.569912	-2.361035
90	9	0	-4.177312	-4.089686	-1.990298
91	9	0	-2.103769	-4.469785	-1.488845
92	1	0	4.370142	2.525602	-1.378961
93	1	0	1.320595	-0.669756	0.366517

TS for [1,2]-hydrogen shift

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.720131	-1.847308	-0.829297
2	6	0	-0.854264	-0.812438	-1.308374
3	6	0	-1.329504	-3.103328	-0.189636
4	6	0	-1.948731	-3.568739	0.978996
5	6	0	-0.244161	-3.819638	-0.716321
6	6	0	-1.488587	-4.722883	1.602862
7	1	0	-2.765082	-3.008535	1.423463
8	6	0	0.213596	-4.970376	-0.084818
9	1	0	0.238712	-3.469358	-1.623913
10	6	0	-0.408040	-5.427481	1.075925
11	1	0	-1.970768	-5.065737	2.512911
12	1	0	1.052929	-5.515322	-0.505898
13	6	0	-1.728398	0.206382	-1.725033
14	1	0	-1.029869	-0.653953	-2.576714
15	6	0	-1.514872	1.597244	-2.147354
16	6	0	-2.337983	2.597703	-1.624965
17	6	0	-0.492567	1.918603	-3.046523
18	6	0	-2.133467	3.919562	-2.007324
19	1	0	-3.109674	2.347004	-0.905633
20	6	0	-0.296411	3.241579	-3.418784
21	1	0	0.133976	1.134598	-3.462456
22	6	0	-1.118007	4.243040	-2.902646
23	1	0	-2.766534	4.697932	-1.594797
24	1	0	0.495105	3.489719	-4.118319
25	8	0	-3.018716	-0.172001	-1.549156
26	7	0	-3.007754	-1.422968	-0.944828
27	6	0	-4.181520	-2.001841	-0.713584
28	1	0	-4.096652	-3.060547	-0.509546
29	6	0	-5.473577	-1.376005	-0.687636
30	6	0	-5.722246	0.015023	-0.688357
31	6	0	-6.584279	-2.249650	-0.610578
32	6	0	-7.016396	0.500977	-0.629540
33	1	0	-4.906664	0.723701	-0.712911
34	6	0	-7.876507	-1.769602	-0.555571
35	1	0	-6.414290	-3.321567	-0.597396
36	6	0	-8.083239	-0.390762	-0.570864
37	1	0	-7.203084	1.567768	-0.622764
38	1	0	-8.720267	-2.446187	-0.502344
39	79	0	1.167466	-0.611303	-0.886914
40	15	0	3.446646	-0.523033	-0.431654
41	6	0	4.359785	-1.676067	-1.517564

42	6	0	3.872023	-2.984313	-1.635591
43	6	0	5.510151	-1.302141	-2.214116
44	6	0	4.533157	-3.906933	-2.437535
45	1	0	2.975380	-3.279749	-1.095526
46	6	0	6.166081	-2.229375	-3.022953
47	1	0	5.898736	-0.292137	-2.129661
48	6	0	5.680716	-3.528841	-3.134752
49	1	0	4.151225	-4.919486	-2.522379
50	1	0	7.058985	-1.932238	-3.563944
51	1	0	6.193755	-4.248013	-3.765660
52	6	0	4.196158	1.114251	-0.693830
53	6	0	5.321350	1.536628	0.018019
54	6	0	3.617437	1.961069	-1.644250
55	6	0	5.860629	2.797253	-0.221219
56	1	0	5.770638	0.891949	0.767082
57	6	0	4.160385	3.219369	-1.881771
58	1	0	2.730192	1.643220	-2.185619
59	6	0	5.281078	3.638782	-1.168521
60	1	0	6.730464	3.124715	0.339333
61	1	0	3.699275	3.875979	-2.612861
62	1	0	5.699568	4.624715	-1.345596
63	6	0	3.858729	-1.066838	1.257966
64	6	0	5.075354	-1.693109	1.548721
65	6	0	2.921601	-0.862554	2.275774
66	6	0	5.352274	-2.101877	2.850076
67	1	0	5.803389	-1.867468	0.761789
68	6	0	3.201888	-1.276038	3.574023
69	1	0	1.980723	-0.371531	2.053539
70	6	0	4.416157	-1.895154	3.861701
71	1	0	6.297339	-2.587547	3.071921
72	1	0	2.466862	-1.117452	4.356151
73	1	0	4.632435	-2.220780	4.874574
74	7	0	-0.026624	1.478551	1.467938
75	16	0	-1.440287	1.105893	2.108790
76	8	0	-2.018630	2.059006	3.043980
77	8	0	-2.303170	0.561962	1.064810
78	16	0	0.962522	2.628168	1.989072
79	8	0	0.650021	3.217230	3.283475
80	8	0	2.333335	2.219006	1.721258
81	7	0	-9.438167	0.125023	-0.516965
82	8	0	-10.362421	-0.678716	-0.457821
83	8	0	-9.598072	1.340527	-0.533842
84	1	0	-0.963997	5.276056	-3.197556
85	1	0	-0.052373	-6.327654	1.567093
86	6	0	-0.986087	-0.367656	3.128043
87	6	0	0.633161	3.956686	0.751102
88	9	0	-0.137717	-0.011856	4.091825
89	9	0	-2.079639	-0.886767	3.680810
90	9	0	-0.405392	-1.300280	2.374669
91	9	0	1.406152	5.009206	1.010790
92	9	0	-0.642444	4.332922	0.808537
93	9	0	0.903142	3.521420	-0.476541

TS6d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.342330	-0.353839	-0.829890
2	6	0	-1.679448	-0.684484	0.361933
3	6	0	-2.341024	-1.277982	-2.005740
4	6	0	-3.473326	-1.338765	-2.826493
5	6	0	-1.234218	-2.076454	-2.312667

6	6	0	-3.517021	-2.222126	-3.899120
7	1	0	-4.329328	-0.702915	-2.627919
8	6	0	-1.278032	-2.952791	-3.391714
9	1	0	-0.330810	-2.001870	-1.720491
10	6	0	-2.421578	-3.035056	-4.181284
11	1	0	-4.407181	-2.269087	-4.517956
12	1	0	-0.415662	-3.570630	-3.615891
13	6	0	-1.812686	0.121176	1.595932
14	6	0	-0.988613	-0.231373	2.807439
15	6	0	-0.806126	0.778613	3.760180
16	6	0	-0.367656	-1.472437	3.002331
17	6	0	-0.015317	0.562684	4.880922
18	1	0	-1.289598	1.735331	3.597277
19	6	0	0.393697	-1.697145	4.146061
20	1	0	-0.459741	-2.273433	2.275389
21	6	0	0.586863	-0.679724	5.076910
22	1	0	0.140891	1.363160	5.597373
23	1	0	0.853408	-2.666819	4.301467
24	8	0	-2.564140	1.092270	1.654998
25	7	0	-2.907076	0.837115	-1.077702
26	6	0	-4.026820	1.412056	-0.972107
27	6	0	-5.274331	0.874603	-0.394379
28	6	0	-5.351229	-0.376805	0.229877
29	6	0	-6.411050	1.686561	-0.469189
30	6	0	-6.554130	-0.818947	0.757977
31	1	0	-4.477685	-1.014608	0.303520
32	6	0	-7.620899	1.258534	0.057844
33	1	0	-6.346253	2.659754	-0.946065
34	6	0	-7.667737	0.008258	0.658982
35	1	0	-6.631661	-1.785383	1.239085
36	1	0	-8.508729	1.874918	0.003663
37	79	0	0.528138	0.163344	-0.144642
38	15	0	1.575502	2.178637	-0.646163
39	6	0	2.689248	2.143881	-2.086609
40	6	0	2.466571	1.192962	-3.085201
41	6	0	3.723415	3.076305	-2.238468
42	6	0	3.269265	1.169598	-4.221186
43	1	0	1.672006	0.461152	-2.966436
44	6	0	4.528106	3.046374	-3.373359
45	1	0	3.905609	3.818951	-1.467836
46	6	0	4.301824	2.093352	-4.364420
47	1	0	3.094377	0.422866	-4.989051
48	1	0	5.331447	3.767990	-3.482639
49	1	0	4.933299	2.068266	-5.247195
50	6	0	0.347725	3.488648	-1.009475
51	6	0	-0.907427	3.428360	-0.394290
52	6	0	0.647629	4.568035	-1.845609
53	6	0	-1.842080	4.437735	-0.602928
54	1	0	-1.156606	2.591639	0.248986
55	6	0	-0.293096	5.571839	-2.060602
56	1	0	1.613466	4.634000	-2.335192
57	6	0	-1.537605	5.509906	-1.438180
58	1	0	-2.809482	4.381863	-0.113281
59	1	0	-0.049342	6.403099	-2.714665
60	1	0	-2.270733	6.292175	-1.608805
61	6	0	2.552966	2.844001	0.754696
62	6	0	1.968451	3.742861	1.654236
63	6	0	3.854334	2.381268	0.993480
64	6	0	2.677375	4.176073	2.770898
65	1	0	0.961616	4.112208	1.490852
66	6	0	4.558127	2.823685	2.109830
67	1	0	4.321221	1.665352	0.322197
68	6	0	3.972178	3.719112	3.000334
69	1	0	2.214580	4.875340	3.460118
70	1	0	5.563817	2.456123	2.287018

71	1	0	4.522284	4.057313	3.873092
72	7	0	1.959261	-2.036401	0.181594
73	16	0	1.469071	-3.579062	0.304295
74	8	0	2.145581	-4.368625	1.320701
75	8	0	0.011553	-3.570819	0.280169
76	16	0	3.524531	-1.651886	0.355456
77	8	0	4.428593	-2.788526	0.261480
78	8	0	3.816126	-0.459536	-0.423220
79	7	0	-8.944542	-0.460300	1.210865
80	8	0	-9.903229	0.295783	1.157040
81	8	0	-8.982165	-1.582773	1.692098
82	1	0	1.204433	-0.852698	5.952951
83	1	0	-2.453049	-3.719382	-5.023379
84	6	0	1.927755	-4.345538	-1.335729
85	6	0	3.624140	-1.078564	2.114329
86	9	0	1.895827	-3.421027	-2.296523
87	9	0	3.135309	-4.885671	-1.293049
88	9	0	1.037568	-5.291204	-1.613521
89	9	0	4.812833	-0.508808	2.300636
90	9	0	3.497666	-2.103429	2.946522
91	9	0	2.672128	-0.185996	2.374238
92	1	0	-4.081094	2.440350	-1.332001
93	1	0	-1.357970	-1.720201	0.431469

11d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.272662	-1.166473	0.146534
2	6	0	-2.240824	-0.230403	0.316808
3	6	0	-1.595802	-2.615910	0.069354
4	6	0	-0.810853	-3.471386	-0.713653
5	6	0	-2.669321	-3.150780	0.792224
6	6	0	-1.109619	-4.827330	-0.790481
7	1	0	0.027378	-3.065734	-1.269616
8	6	0	-2.961698	-4.507832	0.717146
9	1	0	-3.263594	-2.509286	1.435199
10	6	0	-2.185890	-5.349533	-0.077226
11	1	0	-0.499204	-5.477274	-1.409469
12	1	0	-3.792251	-4.910180	1.288455
13	6	0	-2.043060	1.226224	0.373214
14	6	0	-3.218421	2.092072	0.014642
15	6	0	-4.276661	1.639968	-0.780647
16	6	0	-3.224111	3.414419	0.471888
17	6	0	-5.324851	2.496233	-1.106019
18	1	0	-4.277980	0.627114	-1.170338
19	6	0	-4.276718	4.264587	0.157887
20	1	0	-2.393767	3.760573	1.078367
21	6	0	-5.329919	3.805837	-0.632590
22	1	0	-6.136795	2.140163	-1.732123
23	1	0	-4.277255	5.285521	0.526556
24	8	0	-0.989570	1.759276	0.710701
25	7	0	0.058881	-0.870417	-0.121391
26	6	0	0.827152	-0.367321	0.756981
27	1	0	0.495691	-0.181877	1.781563
28	6	0	2.224146	-0.015032	0.445273
29	6	0	2.750487	-0.198487	-0.838897
30	6	0	3.026391	0.516762	1.458113
31	6	0	4.064365	0.144114	-1.110425
32	1	0	2.120652	-0.608447	-1.620530
33	6	0	4.345511	0.865658	1.201753

34	1	0	2.616167	0.660213	2.452763
35	6	0	4.838996	0.671212	-0.081228
36	1	0	4.487718	0.009867	-2.097532
37	1	0	4.979048	1.279244	1.975789
38	7	0	6.230320	1.035876	-0.363493
39	8	0	6.900717	1.497295	0.549255
40	8	0	6.651749	0.860013	-1.497929
41	1	0	-6.151850	4.469926	-0.881734
42	1	0	-2.415334	-6.408976	-0.134154
43	1	0	-3.266032	-0.581321	0.330859

Ts7d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.651128	-1.104951	0.369212
2	6	0	-2.156241	0.178567	0.578154
3	6	0	-2.547519	-2.268019	0.139816
4	6	0	-2.063086	-3.390036	-0.543273
5	6	0	-3.864732	-2.280047	0.613970
6	6	0	-2.883477	-4.489757	-0.765233
7	1	0	-1.040206	-3.386588	-0.903293
8	6	0	-4.680260	-3.386024	0.401007
9	1	0	-4.253392	-1.435163	1.173051
10	6	0	-4.194726	-4.491180	-0.294224
11	1	0	-2.497817	-5.348461	-1.305767
12	1	0	-5.696478	-3.385201	0.782200
13	6	0	-1.338849	1.322546	0.352925
14	6	0	-1.967613	2.624358	-0.017256
15	6	0	-3.229312	2.707635	-0.618076
16	6	0	-1.253391	3.801048	0.239601
17	6	0	-3.767184	3.947460	-0.946623
18	1	0	-3.784738	1.806814	-0.856458
19	6	0	-1.796111	5.038646	-0.083148
20	1	0	-0.274507	3.733808	0.701845
21	6	0	-3.054949	5.113714	-0.676266
22	1	0	-4.741806	4.002017	-1.420835
23	1	0	-1.238438	5.945226	0.129139
24	8	0	-0.074990	1.307963	0.394316
25	7	0	-0.333015	-1.321258	0.228143
26	6	0	0.469333	-0.504220	0.883970
27	1	0	0.222762	-0.240087	1.916290
28	6	0	1.909155	-0.456597	0.541791
29	6	0	2.388440	-1.065387	-0.620685
30	6	0	2.786363	0.222029	1.390212
31	6	0	3.737065	-1.003752	-0.935280
32	1	0	1.697284	-1.590457	-1.270265
33	6	0	4.138577	0.296542	1.088027
34	1	0	2.408162	0.696569	2.290034
35	6	0	4.587661	-0.320874	-0.072567
36	1	0	4.128662	-1.471718	-1.829402
37	1	0	4.833243	0.817458	1.734288
38	7	0	6.014625	-0.252102	-0.399155
39	8	0	6.751544	0.354030	0.365906
40	8	0	6.398194	-0.804274	-1.420717
41	1	0	-3.479275	6.080045	-0.930531
42	1	0	-4.834290	-5.351676	-0.464187
43	1	0	-3.226526	0.328992	0.578591

4t

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.957314	0.074364	1.383530
2	6	0	0.687415	0.464033	1.584868
3	6	0	2.485218	-1.199177	0.852334
4	6	0	3.305056	-2.015118	1.638011
5	6	0	2.141351	-1.606747	-0.438665
6	6	0	3.787836	-3.216216	1.128965
7	1	0	3.572932	-1.703170	2.643650
8	6	0	2.617438	-2.813167	-0.942215
9	1	0	1.522074	-0.960880	-1.049483
10	6	0	3.446738	-3.616398	-0.162580
11	1	0	4.429604	-3.841332	1.741734
12	1	0	2.345306	-3.119983	-1.947171
13	6	0	0.708528	1.799859	2.246257
14	8	0	2.135302	2.065768	2.486496
15	7	0	2.845937	1.115378	1.827859
16	6	0	4.115691	1.326711	1.731258
17	6	0	5.048429	0.513608	0.945302
18	6	0	4.798530	0.237338	-0.403453
19	6	0	6.218717	0.056403	1.560112
20	6	0	5.686749	-0.549126	-1.121253
21	1	0	3.913718	0.638411	-0.886141
22	6	0	7.109455	-0.734985	0.850638
23	1	0	6.417400	0.297731	2.598882
24	6	0	6.817871	-1.031453	-0.475108
25	1	0	5.504383	-0.787710	-2.161063
26	1	0	8.009247	-1.120043	1.312782
27	79	0	-0.957333	-0.552521	0.902626
28	15	0	-2.711923	-1.806985	0.003123
29	6	0	-2.062980	-3.094484	-1.118342
30	6	0	-0.923000	-3.800734	-0.714430
31	6	0	-2.658248	-3.388994	-2.347229
32	6	0	-0.393633	-4.797566	-1.526553
33	1	0	-0.443621	-3.565222	0.232531
34	6	0	-2.119158	-4.382900	-3.161599
35	1	0	-3.538325	-2.844552	-2.674514
36	6	0	-0.990244	-5.087979	-2.752646
37	1	0	0.491953	-5.337428	-1.206433
38	1	0	-2.583880	-4.603718	-4.117378
39	1	0	-0.571746	-5.860119	-3.390781
40	6	0	-3.701603	-2.697427	1.250065
41	6	0	-3.987788	-2.043372	2.454096
42	6	0	-4.198847	-3.983972	1.024687
43	6	0	-4.770582	-2.668803	3.418920
44	1	0	-3.597638	-1.044853	2.635253
45	6	0	-4.977458	-4.608325	1.996329
46	1	0	-3.979759	-4.500314	0.094883
47	6	0	-5.264269	-3.952271	3.191043
48	1	0	-4.989662	-2.156337	4.350341
49	1	0	-5.359427	-5.608602	1.818241
50	1	0	-5.869891	-4.442371	3.947064
51	6	0	-3.909724	-0.846193	-0.977183
52	6	0	-5.239623	-1.251844	-1.130836
53	6	0	-3.460321	0.312251	-1.617195
54	6	0	-6.103755	-0.505809	-1.926935
55	1	0	-5.601723	-2.145636	-0.631488
56	6	0	-4.325632	1.053772	-2.414887
57	1	0	-2.436062	0.639899	-1.477419
58	6	0	-5.647411	0.643977	-2.570223
59	1	0	-7.135856	-0.821559	-2.042398
60	1	0	-3.965743	1.956600	-2.897568

61	1	0	-6.326394	1.224930	-3.186782
62	7	0	-0.411308	2.573901	-0.825914
63	16	0	0.745776	2.444695	-1.923804
64	8	0	0.952851	3.599280	-2.786601
65	8	0	1.904646	1.834116	-1.282152
66	16	0	-1.653805	3.584660	-0.904867
67	8	0	-2.059812	3.995946	-2.242858
68	8	0	-2.668344	3.111292	0.026433
69	1	0	3.827280	-4.552647	-0.559111
70	6	0	0.115134	1.126565	-3.063095
71	6	0	-1.001948	5.120742	-0.102294
72	9	0	-1.001919	1.521458	-3.662610
73	9	0	1.040327	0.873594	-3.984938
74	9	0	-0.137165	-0.004258	-2.397631
75	9	0	0.057356	5.588008	-0.751999
76	9	0	-0.652034	4.865784	1.159745
77	9	0	-1.955973	6.048056	-0.100237
78	1	0	4.476361	2.194633	2.274591
79	1	0	0.375863	2.567102	1.537273
80	6	0	-0.040768	1.957778	3.585951
81	6	0	0.382579	3.286925	4.231252
82	1	0	-0.201484	3.456410	5.141457
83	1	0	1.441029	3.284715	4.506211
84	1	0	0.205258	4.129339	3.555005
85	6	0	0.284531	0.793299	4.526849
86	1	0	-0.082706	-0.157077	4.125110
87	1	0	1.364644	0.703667	4.687462
88	1	0	-0.187640	0.953682	5.501501
89	6	0	-1.546370	2.011233	3.296994
90	1	0	-1.787304	2.810518	2.589440
91	1	0	-1.912695	1.069645	2.874927
92	1	0	-2.091413	2.198993	4.228076
93	7	0	7.745829	-1.884353	-1.224544
94	8	0	8.738924	-2.297940	-0.644156
95	8	0	7.476018	-2.139900	-2.388599

Ts2t

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.909584	-0.393839	1.432819
2	6	0	0.605767	0.062350	1.542163
3	6	0	2.378596	-1.732509	1.034841
4	6	0	3.266781	-2.456427	1.840646
5	6	0	1.905120	-2.320673	-0.143422
6	6	0	3.674707	-3.732626	1.470247
7	1	0	3.642758	-2.017025	2.760014
8	6	0	2.305965	-3.602903	-0.507026
9	1	0	1.223410	-1.766424	-0.779494
10	6	0	3.196930	-4.311312	0.295136
11	1	0	4.366320	-4.278706	2.104280
12	1	0	1.926395	-4.042422	-1.424492
13	6	0	0.662233	1.344135	2.126967
14	8	0	2.035657	1.601338	2.468297
15	7	0	2.766744	0.582076	1.936894
16	6	0	4.075136	0.742883	1.955800
17	6	0	4.992857	0.023683	1.094704
18	6	0	4.665322	-0.312665	-0.232120
19	6	0	6.267120	-0.305912	1.586507
20	6	0	5.560826	-1.008771	-1.024074
21	1	0	3.711987	-0.011068	-0.649027
22	6	0	7.170693	-1.002181	0.802019

23	1	0	6.536043	-0.032429	2.601564
24	6	0	6.797895	-1.357838	-0.490831
25	1	0	5.311476	-1.275016	-2.043365
26	1	0	8.145641	-1.278944	1.182999
27	79	0	-1.076111	-0.782050	0.736222
28	15	0	-2.996545	-1.684073	-0.235607
29	6	0	-2.723880	-3.344331	-0.938347
30	6	0	-1.713312	-4.142333	-0.389423
31	6	0	-3.492822	-3.834148	-1.999290
32	6	0	-1.480117	-5.418912	-0.891922
33	1	0	-1.104654	-3.762082	0.427129
34	6	0	-3.255367	-5.111377	-2.499225
35	1	0	-4.272302	-3.219966	-2.440228
36	6	0	-2.250469	-5.903339	-1.946944
37	1	0	-0.690617	-6.028941	-0.464510
38	1	0	-3.853178	-5.485590	-3.324218
39	1	0	-2.064327	-6.896727	-2.343150
40	6	0	-4.363890	-1.833107	0.963563
41	6	0	-4.602377	-0.741322	1.809105
42	6	0	-5.164347	-2.972737	1.060751
43	6	0	-5.638142	-0.789609	2.734776
44	1	0	-3.978759	0.146912	1.740871
45	6	0	-6.197086	-3.018496	1.995708
46	1	0	-4.986580	-3.825337	0.412678
47	6	0	-6.434798	-1.930315	2.830685
48	1	0	-5.818657	0.060478	3.385193
49	1	0	-6.814701	-3.908027	2.069801
50	1	0	-7.239555	-1.970376	3.558225
51	6	0	-3.654738	-0.664303	-1.595865
52	6	0	-5.024529	-0.584237	-1.865022
53	6	0	-2.748196	0.042668	-2.393277
54	6	0	-5.478830	0.191345	-2.928193
55	1	0	-5.736824	-1.120402	-1.244786
56	6	0	-3.206721	0.814429	-3.455748
57	1	0	-1.684162	-0.002322	-2.178246
58	6	0	-4.571853	0.889040	-3.723200
59	1	0	-6.543142	0.253392	-3.132035
60	1	0	-2.498662	1.367980	-4.062877
61	1	0	-4.930253	1.498303	-4.547095
62	7	0	0.197538	2.690072	-0.187347
63	16	0	1.496452	2.914325	-1.155308
64	8	0	1.452960	4.190254	-1.841861
65	8	0	2.659287	2.502045	-0.394286
66	16	0	-1.259507	3.425746	-0.401976
67	8	0	-1.871497	3.072586	-1.666187
68	8	0	-1.968358	3.265552	0.850634
69	1	0	3.519425	-5.307002	0.007078
70	6	0	1.296512	1.602159	-2.452656
71	6	0	-0.817448	5.248291	-0.520928
72	9	0	0.272769	1.868468	-3.245321
73	9	0	2.414275	1.554128	-3.165234
74	9	0	1.103524	0.422686	-1.866266
75	9	0	-0.880486	5.640079	-1.781515
76	9	0	0.405368	5.462192	-0.053778
77	9	0	-1.691591	5.932368	0.201789
78	1	0	4.431898	1.511698	2.629403
79	1	0	0.407069	2.065584	0.870308
80	6	0	-0.318056	1.989120	3.124277
81	6	0	-0.389152	3.505686	2.866258
82	1	0	-0.597925	4.014254	3.784230
83	1	0	0.547217	3.845255	2.475353
84	1	0	-1.166147	3.711266	2.159918
85	6	0	0.171488	1.735442	4.562190
86	1	0	-0.434436	0.979973	5.017187
87	1	0	1.190495	1.409829	4.539809

88	1	0	0.098542	2.640268	5.128644
89	6	0	-1.716791	1.371218	2.941692
90	1	0	-1.755844	0.845910	2.010335
91	1	0	-1.913498	0.690631	3.743570
92	1	0	-2.452879	2.147793	2.944310
93	7	0	7.739570	-2.125603	-1.318288
94	8	0	8.729878	-2.561004	-0.800470
95	8	0	7.479931	-2.285932	-2.478155

4a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.504947	1.651345	1.093245
2	6	0	-0.832558	0.471956	1.193872
3	6	0	-0.989534	3.006643	0.813017
4	6	0	-1.169393	4.041892	1.738101
5	6	0	-0.297984	3.269629	-0.372158
6	6	0	-0.675282	5.314433	1.476240
7	1	0	-1.706417	3.853611	2.663402
8	6	0	0.199837	4.543595	-0.630723
9	1	0	-0.178262	2.483437	-1.109689
10	6	0	0.009753	5.570764	0.289405
11	1	0	-0.825967	6.107836	2.201594
12	1	0	0.721826	4.732059	-1.563828
13	6	0	-1.789424	-0.520798	1.657161
14	6	0	-1.544118	-1.619974	2.635642
15	6	0	-2.621921	-2.440743	2.986911
16	6	0	-0.282397	-1.896185	3.166638
17	6	0	-2.439956	-3.517858	3.846948
18	1	0	-3.605439	-2.240962	2.573454
19	6	0	-0.098241	-2.986993	4.012617
20	1	0	0.559875	-1.258919	2.915127
21	6	0	-1.173877	-3.800844	4.356875
22	1	0	-3.286356	-4.145506	4.108986
23	1	0	0.889911	-3.191935	4.413992
24	8	0	-3.018452	0.189214	1.967439
25	7	0	-2.857920	1.460248	1.506690
26	6	0	-3.930168	2.194712	1.496009
27	6	0	-4.085597	3.449362	0.770235
28	6	0	-3.596223	3.610080	-0.534089
29	6	0	-4.788300	4.497762	1.379081
30	6	0	-3.775068	4.817706	-1.196565
31	1	0	-3.097075	2.785307	-1.031803
32	6	0	-4.962897	5.702038	0.707896
33	1	0	-5.180759	4.369676	2.383619
34	6	0	-4.449866	5.868914	-0.577685
35	1	0	-3.386583	4.934930	-2.203244
36	1	0	-5.499368	6.512256	1.191765
37	79	0	1.089172	0.145683	0.543092
38	15	0	3.321733	0.012903	-0.156120
39	6	0	3.662382	1.080271	-1.598613
40	6	0	3.138856	2.379561	-1.584364
41	6	0	4.442298	0.662145	-2.679044
42	6	0	3.403644	3.252230	-2.633240
43	1	0	2.525607	2.712690	-0.750861
44	6	0	4.690551	1.535923	-3.736244
45	1	0	4.851958	-0.342224	-2.707142
46	6	0	4.176396	2.829233	-3.713752
47	1	0	3.002721	4.260824	-2.607947
48	1	0	5.288938	1.201979	-4.578007
49	1	0	4.373731	3.506845	-4.538611

50	6	0	4.452605	0.613952	1.147296
51	6	0	4.291761	0.119870	2.447606
52	6	0	5.479936	1.519617	0.873297
53	6	0	5.158385	0.521825	3.458237
54	1	0	3.492592	-0.583454	2.669575
55	6	0	6.339774	1.926466	1.891327
56	1	0	5.614599	1.906691	-0.131821
57	6	0	6.182345	1.426842	3.181052
58	1	0	5.034042	0.131255	4.463165
59	1	0	7.134958	2.631953	1.671683
60	1	0	6.853904	1.745539	3.972150
61	6	0	3.970145	-1.628694	-0.614808
62	6	0	5.324982	-1.934941	-0.439152
63	6	0	3.107519	-2.588628	-1.154189
64	6	0	5.811534	-3.186248	-0.803395
65	1	0	6.002623	-1.197188	-0.020591
66	6	0	3.601315	-3.839833	-1.516026
67	1	0	2.056932	-2.355763	-1.312281
68	6	0	4.949370	-4.140333	-1.338203
69	1	0	6.863610	-3.415219	-0.666468
70	1	0	2.924863	-4.586398	-1.917345
71	1	0	5.327325	-5.119269	-1.616384
72	7	0	-2.331282	-1.807886	-0.702212
73	16	0	-3.215733	-1.004450	-1.788349
74	8	0	-4.061830	-1.855632	-2.609666
75	8	0	-3.774657	0.150459	-1.103598
76	16	0	-1.795856	-3.322259	-0.904968
77	8	0	-1.490722	-3.648755	-2.289329
78	8	0	-0.814384	-3.554742	0.139952
79	1	0	-1.028231	-4.648463	5.019433
80	1	0	0.389793	6.566486	0.083018
81	6	0	-1.939634	-0.284880	-2.933474
82	6	0	-3.273006	-4.378865	-0.450022
83	9	0	-1.425257	-1.212865	-3.723719
84	9	0	-2.521024	0.657484	-3.671439
85	9	0	-0.953415	0.271865	-2.229289
86	9	0	-3.908598	-4.769811	-1.544444
87	9	0	-4.112749	-3.699102	0.322287
88	9	0	-2.840468	-5.447225	0.210125
89	1	0	-4.761522	1.778148	2.054386
90	1	0	-2.028725	-1.112768	0.584489
91	1	0	-4.589843	6.809687	-1.102374

Ts2a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.135366	-1.023544	1.123160
2	6	0	1.043418	-0.169791	1.247043
3	6	0	2.134085	-2.453013	0.771572
4	6	0	2.715126	-3.408914	1.614994
5	6	0	1.509275	-2.884743	-0.404605
6	6	0	2.672032	-4.759334	1.287360
7	1	0	3.207396	-3.091627	2.529512
8	6	0	1.457541	-4.237966	-0.725959
9	1	0	1.075522	-2.151691	-1.076402
10	6	0	2.041764	-5.180292	0.116967
11	1	0	3.129859	-5.486380	1.951088
12	1	0	0.965856	-4.552223	-1.641699
13	6	0	1.525437	1.038445	1.767478
14	6	0	0.887812	2.008408	2.680014
15	6	0	1.580222	3.176635	3.029170

16	6	0	-0.409411	1.825300	3.178123
17	6	0	0.992716	4.130800	3.853273
18	1	0	2.580600	3.342713	2.640806
19	6	0	-1.002455	2.792070	3.983083
20	1	0	-0.954147	0.918128	2.934892
21	6	0	-0.304730	3.948029	4.327652
22	1	0	1.546614	5.027971	4.113325
23	1	0	-2.010346	2.631832	4.355330
24	8	0	2.922224	0.871573	2.044027
25	7	0	3.275221	-0.365365	1.579037
26	6	0	4.564847	-0.634745	1.614700
27	6	0	5.221213	-1.679788	0.844235
28	6	0	4.842747	-2.000518	-0.469924
29	6	0	6.307474	-2.359182	1.417436
30	6	0	5.506240	-3.001322	-1.168577
31	1	0	4.041248	-1.449214	-0.947659
32	6	0	6.970639	-3.356597	0.711943
33	1	0	6.618609	-2.108600	2.427786
34	6	0	6.565722	-3.689961	-0.579751
35	1	0	5.197148	-3.239767	-2.181763
36	1	0	7.802176	-3.879526	1.174626
37	79	0	-0.869782	-0.558994	0.615738
38	15	0	-3.030392	-1.051248	-0.123858
39	6	0	-3.125258	-2.697189	-0.905775
40	6	0	-2.266392	-3.699172	-0.437843
41	6	0	-4.025097	-2.984255	-1.936409
42	6	0	-2.313049	-4.975271	-0.989878
43	1	0	-1.554284	-3.478677	0.353335
44	6	0	-4.065610	-4.261977	-2.488738
45	1	0	-4.691914	-2.214253	-2.312364
46	6	0	-3.212105	-5.256925	-2.016603
47	1	0	-1.639491	-5.743588	-0.623408
48	1	0	-4.763688	-4.478332	-3.291230
49	1	0	-3.244358	-6.250671	-2.452432
50	6	0	-4.234426	-1.069228	1.248200
51	6	0	-4.189196	-0.011444	2.165623
52	6	0	-5.183770	-2.081167	1.404122
53	6	0	-5.090712	0.034176	3.222806
54	1	0	-3.448676	0.776740	2.051036
55	6	0	-6.080487	-2.034633	2.470155
56	1	0	-5.226724	-2.906391	0.700044
57	6	0	-6.035946	-0.979494	3.377204
58	1	0	-5.051077	0.857227	3.929422
59	1	0	-6.814384	-2.825507	2.589162
60	1	0	-6.734899	-0.947395	4.207250
61	6	0	-3.707437	0.129746	-1.337096
62	6	0	-5.075611	0.411668	-1.405339
63	6	0	-2.826245	0.757134	-2.224173
64	6	0	-5.554175	1.307405	-2.357505
65	1	0	-5.767421	-0.062874	-0.715833
66	6	0	-3.308472	1.652037	-3.173714
67	1	0	-1.761345	0.554042	-2.168488
68	6	0	-4.672494	1.927248	-3.240748
69	1	0	-6.616656	1.524363	-2.405243
70	1	0	-2.614866	2.143119	-3.848125
71	1	0	-5.048472	2.630957	-3.976971
72	7	0	1.473311	2.355581	-0.638404
73	16	0	2.656522	1.925052	-1.708244
74	8	0	3.024760	3.018934	-2.579513
75	8	0	3.639617	1.213974	-0.918857
76	16	0	0.130545	3.219482	-1.047274
77	8	0	-0.131252	3.111864	-2.469722
78	8	0	-0.885090	2.930292	-0.058522
79	1	0	-0.766628	4.698500	4.961792
80	1	0	2.010807	-6.235361	-0.137086

81	6	0	1.854783	0.632467	-2.812455
82	6	0	0.647067	4.972663	-0.726263
83	9	0	1.489726	1.175802	-3.957012
84	9	0	2.749838	-0.319625	-3.036341
85	9	0	0.793759	0.099710	-2.214326
86	9	0	1.611405	5.329156	-1.557040
87	9	0	1.066376	5.087313	0.524111
88	9	0	-0.415144	5.745059	-0.914718
89	1	0	5.142907	0.031397	2.242905
90	1	0	1.467257	1.772203	0.391185
91	1	0	7.078857	-4.474330	-1.127455

4t complex with pyridine

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.097081	0.764213	0.760930
2	6	0	1.305290	0.923369	-0.310285
3	6	0	1.772216	0.668033	2.199356
4	6	0	1.894704	-0.547024	2.880829
5	6	0	1.267689	1.789377	2.865807
6	6	0	1.518111	-0.635987	4.217330
7	1	0	2.257142	-1.425821	2.355657
8	6	0	0.888113	1.695378	4.201523
9	1	0	1.162838	2.727595	2.329110
10	6	0	1.016297	0.483577	4.878443
11	1	0	1.602559	-1.584648	4.737004
12	1	0	0.490097	2.566615	4.711978
13	6	0	2.171853	0.952549	-1.524442
14	1	0	2.126328	1.931650	-2.015083
15	8	0	3.548656	0.838826	-0.994408
16	7	0	3.468989	0.687251	0.340251
17	6	0	4.529401	0.516507	1.058509
18	1	0	4.319431	0.426034	2.118477
19	6	0	5.910992	0.427830	0.617552
20	6	0	6.348475	0.518956	-0.715311
21	6	0	6.852757	0.226845	1.642545
22	6	0	7.699222	0.407717	-1.010000
23	1	0	5.647234	0.677330	-1.521166
24	6	0	8.202278	0.116609	1.354744
25	1	0	6.520226	0.155365	2.672760
26	6	0	8.600396	0.209300	0.027197
27	1	0	8.049068	0.474200	-2.032246
28	1	0	8.931742	-0.038594	2.138999
29	79	0	-0.740307	1.072650	-0.157068
30	15	0	-3.028374	1.146333	0.319710
31	6	0	-3.712879	2.827788	0.499766
32	6	0	-3.064351	3.901183	-0.118968
33	6	0	-4.899741	3.049605	1.207355
34	6	0	-3.605211	5.182080	-0.035446
35	1	0	-2.139483	3.736661	-0.667253
36	6	0	-5.430909	4.331618	1.294223
37	1	0	-5.409832	2.223316	1.693032
38	6	0	-4.784905	5.398268	0.671054
39	1	0	-3.100459	6.010324	-0.521175
40	1	0	-6.349836	4.497727	1.847457
41	1	0	-5.201053	6.398691	0.738791
42	6	0	-4.093902	0.322131	-0.913041
43	6	0	-4.039928	-1.072326	-1.021650
44	6	0	-4.906458	1.053509	-1.782759
45	6	0	-4.802098	-1.726767	-1.982231
46	1	0	-3.410695	-1.655128	-0.356298

47	6	0	-5.661368	0.392757	-2.749803
48	1	0	-4.957868	2.135372	-1.708196
49	6	0	-5.612301	-0.995133	-2.848995
50	1	0	-4.748562	-2.807772	-2.052550
51	1	0	-6.291839	0.966597	-3.421875
52	1	0	-6.204186	-1.507333	-3.601319
53	6	0	-3.367781	0.295219	1.900751
54	6	0	-4.581753	-0.352024	2.153350
55	6	0	-2.372733	0.300850	2.885044
56	6	0	-4.792310	-0.989217	3.372734
57	1	0	-5.359121	-0.375507	1.396015
58	6	0	-2.588910	-0.334020	4.103611
59	1	0	-1.419293	0.786919	2.695214
60	6	0	-3.796832	-0.983079	4.347098
61	1	0	-5.733529	-1.497204	3.557426
62	1	0	-1.803587	-0.334123	4.852668
63	1	0	-3.960474	-1.490273	5.292883
64	7	0	-0.303348	-4.087181	-0.581347
65	16	0	-0.164323	-4.341230	0.986985
66	8	0	-0.912561	-5.483701	1.499512
67	8	0	1.240024	-4.191610	1.344705
68	16	0	-1.591656	-4.516524	-1.437334
69	8	0	-1.426635	-5.789142	-2.130289
70	8	0	-2.880887	-4.247958	-0.802865
71	1	0	0.720136	0.410321	5.920349
72	6	0	-0.961589	-2.864810	1.775877
73	6	0	-1.428486	-3.232780	-2.756453
74	9	0	-2.283230	-2.898108	1.655041
75	9	0	-0.650891	-2.840944	3.071007
76	9	0	-0.505088	-1.750699	1.204021
77	9	0	-2.472485	-3.340289	-3.577034
78	9	0	-0.315347	-3.409275	-3.461691
79	9	0	-1.422015	-2.011028	-2.230774
80	7	0	0.546064	3.840889	-2.143590
81	6	0	-0.308042	4.558831	-2.880127
82	6	0	0.910185	4.340349	-0.956916
83	6	0	-0.819271	5.789621	-2.477243
84	1	0	-0.593929	4.131334	-3.838103
85	6	0	0.453609	5.557561	-0.462709
86	1	0	1.600997	3.734236	-0.374479
87	6	0	-0.425978	6.300685	-1.244372
88	1	0	-1.507806	6.329568	-3.118066
89	1	0	0.786300	5.912784	0.506543
90	1	0	-0.799904	7.258863	-0.897284
91	7	0	10.028635	0.094403	-0.290450
92	8	0	10.807743	-0.072247	0.635882
93	8	0	10.361372	0.172865	-1.463289
94	6	0	1.971045	-0.166417	-2.570651
95	6	0	1.889594	-1.530667	-1.879417
96	1	0	1.000169	-1.614046	-1.250241
97	1	0	1.846749	-2.329700	-2.623616
98	1	0	2.770686	-1.708884	-1.252295
99	6	0	3.154642	-0.146875	-3.549779
100	1	0	3.296336	0.849172	-3.984579
101	1	0	4.086836	-0.448258	-3.062966
102	1	0	2.964487	-0.848198	-4.368425
103	6	0	0.685156	0.137470	-3.350177
104	1	0	-0.187208	0.189422	-2.693144
105	1	0	0.767176	1.091342	-3.882319
106	1	0	0.506840	-0.652895	-4.085656

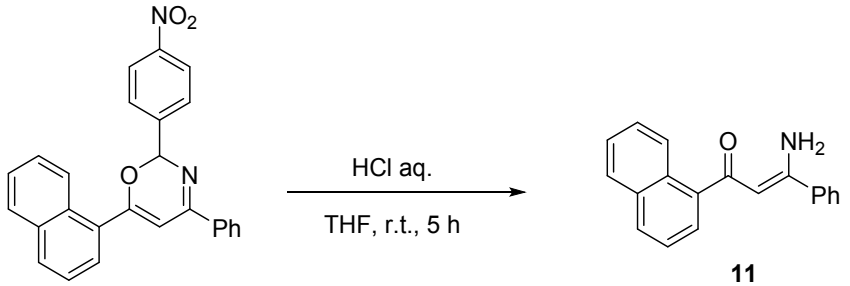
Ts2t-py

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.942839	-0.013782	0.954971
2	6	0	1.095835	0.266953	-0.105373
3	6	0	1.628775	-0.264508	2.371410
4	6	0	2.071409	-1.419374	3.026665
5	6	0	0.809374	0.637812	3.061110
6	6	0	1.695010	-1.666888	4.342710
7	1	0	2.674153	-2.143369	2.488143
8	6	0	0.423943	0.381594	4.373287
9	1	0	0.471003	1.540192	2.559531
10	6	0	0.867351	-0.771496	5.017725
11	1	0	2.033334	-2.573033	4.835402
12	1	0	-0.217349	1.086621	4.893632
13	6	0	1.916916	0.575040	-1.215092
14	1	0	1.880849	1.982856	-1.060749
15	8	0	3.272963	0.268926	-0.816076
16	7	0	3.253153	-0.000570	0.499227
17	6	0	4.396212	-0.115808	1.160861
18	1	0	4.261558	-0.249615	2.224992
19	6	0	5.727708	-0.079715	0.624428
20	6	0	6.078287	-0.009496	-0.743009
21	6	0	6.775417	-0.130411	1.576195
22	6	0	7.407491	0.020155	-1.130666
23	1	0	5.315256	0.009948	-1.506517
24	6	0	8.100089	-0.097790	1.194671
25	1	0	6.528830	-0.194250	2.631292
26	6	0	8.406455	-0.017922	-0.163984
27	1	0	7.671467	0.070654	-2.179727
28	1	0	8.894258	-0.133510	1.929988
29	79	0	-0.929274	0.565166	0.048968
30	15	0	-3.139594	1.298834	0.240410
31	6	0	-3.146513	3.084807	0.641339
32	6	0	-2.237441	3.540043	1.604967
33	6	0	-4.028996	3.988930	0.045328
34	6	0	-2.216291	4.882207	1.969528
35	1	0	-1.544008	2.842839	2.069361
36	6	0	-3.998074	5.334509	0.406076
37	1	0	-4.738675	3.649602	-0.702726
38	6	0	-3.094723	5.782076	1.366717
39	1	0	-1.508449	5.226794	2.716799
40	1	0	-4.684507	6.031910	-0.063545
41	1	0	-3.074039	6.830898	1.645983
42	6	0	-4.052132	1.142217	-1.330301
43	6	0	-5.215843	0.382710	-1.452063
44	6	0	-3.487674	1.733478	-2.468356
45	6	0	-5.809787	0.216342	-2.702211
46	1	0	-5.655428	-0.093928	-0.582157
47	6	0	-4.088978	1.573740	-3.710224
48	1	0	-2.570761	2.311794	-2.384633
49	6	0	-5.250491	0.810441	-3.828967
50	1	0	-6.709588	-0.383911	-2.791417
51	1	0	-3.645609	2.034700	-4.587157
52	1	0	-5.713960	0.675294	-4.801200
53	6	0	-4.161746	0.534911	1.538094
54	6	0	-5.395496	1.087573	1.903166
55	6	0	-3.700082	-0.616437	2.180604
56	6	0	-6.161531	0.481782	2.892510
57	1	0	-5.757630	1.988310	1.415318
58	6	0	-4.470321	-1.219809	3.171740
59	1	0	-2.739725	-1.040279	1.908705
60	6	0	-5.700099	-0.672671	3.525783
61	1	0	-7.118483	0.911090	3.171809
62	1	0	-4.105186	-2.115623	3.663947

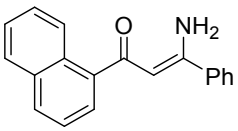
63	1	0	-6.300651	-1.142440	4.298581
64	7	0	-0.562472	-3.112253	-1.004733
65	16	0	0.313013	-3.874127	0.087266
66	8	0	0.340979	-5.326235	-0.040327
67	8	0	1.570739	-3.161260	0.260441
68	16	0	-1.718569	-3.810316	-1.872395
69	8	0	-1.318887	-3.996321	-3.262625
70	8	0	-2.456504	-4.884631	-1.217819
71	1	0	0.568869	-0.972183	6.042069
72	6	0	-0.604383	-3.561943	1.665163
73	6	0	-2.890806	-2.383361	-1.911386
74	9	0	-1.825894	-4.085706	1.615476
75	9	0	0.059088	-4.111049	2.681240
76	9	0	-0.719442	-2.252314	1.890951
77	9	0	-3.981594	-2.742630	-2.584112
78	9	0	-2.342019	-1.334033	-2.517135
79	9	0	-3.247668	-2.040559	-0.674137
80	7	0	1.913109	3.244703	-0.863732
81	6	0	0.765399	3.857580	-0.556244
82	6	0	3.065103	3.919020	-0.932990
83	6	0	0.728726	5.218616	-0.301909
84	1	0	-0.116945	3.223058	-0.513696
85	6	0	3.105064	5.282855	-0.689913
86	1	0	3.947790	3.340110	-1.184322
87	6	0	1.918580	5.939607	-0.371350
88	1	0	-0.211763	5.695960	-0.052750
89	1	0	4.046660	5.815326	-0.748671
90	1	0	1.921922	7.006826	-0.176637
91	7	0	9.797506	0.024281	-0.576327
92	8	0	10.660573	-0.015382	0.293679
93	8	0	10.046574	0.099621	-1.774436
94	6	0	1.717309	0.261582	-2.697015
95	6	0	1.726565	-1.257696	-2.921805
96	1	0	0.915028	-1.738687	-2.369040
97	1	0	1.606120	-1.485186	-3.987192
98	1	0	2.672683	-1.695789	-2.587168
99	6	0	2.845153	0.918055	-3.511211
100	1	0	2.867987	2.003475	-3.361840
101	1	0	3.827154	0.514354	-3.245922
102	1	0	2.687713	0.728440	-4.577846
103	6	0	0.375909	0.846690	-3.157754
104	1	0	-0.463690	0.371188	-2.644776
105	1	0	0.326140	1.927186	-2.979815
106	1	0	0.253259	0.675251	-4.232194

14. Appendix 1. Derivatization of the product 2s



2s **11**
90% yield

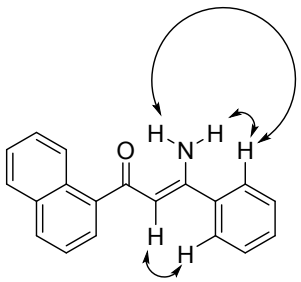
To a solution of **2s** (40.6 mg, 0.1 mmol) in THF (0.4 mL) in a V-vial under argon atmosphere was added Hydrochloric acid (1N concentration, 50 μL). The resulting mixture was stirred at room temperature for 5 h, then saturated ammonium chloride aqueous solution was added. The resulting mixture was extracted with ethyl acetate, and the combined extracts were washed with water and brine, dried over anhydrous Na_2SO_4, and concentrated. The residue was isolated by a flash silica-gel column chromatography with hexane/EtOAc (5:1) as the eluent to afford product **11** (24.6 mg, 0.09 mmol, 90%).

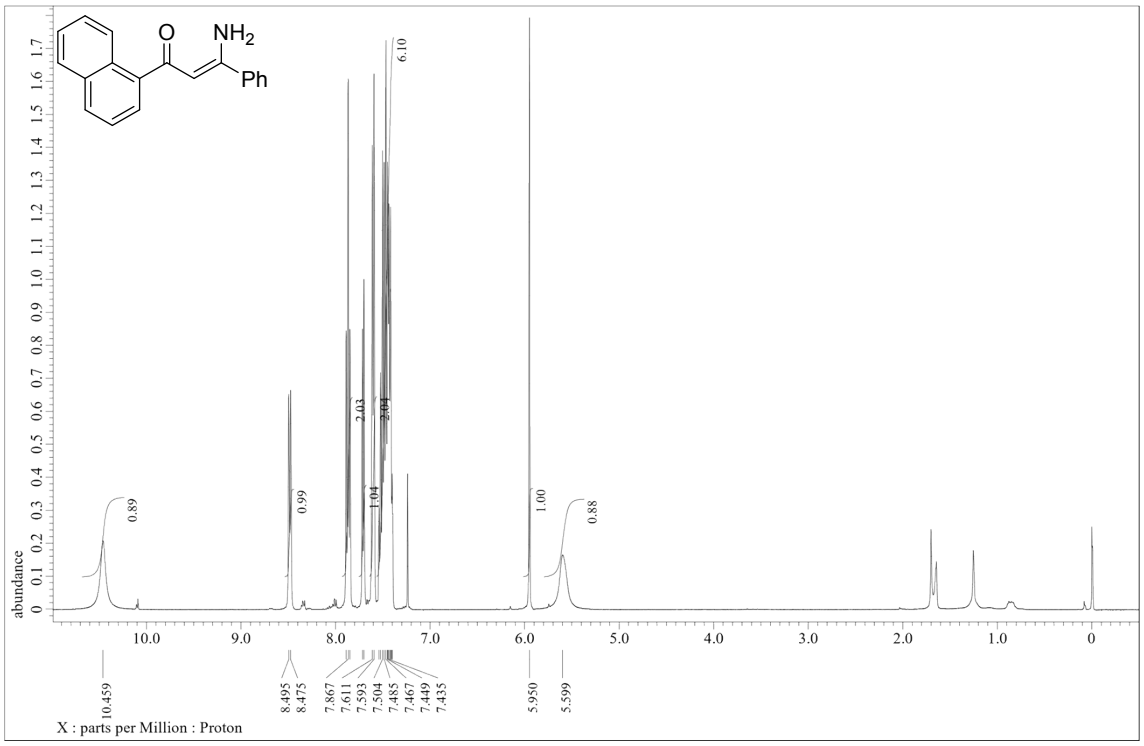


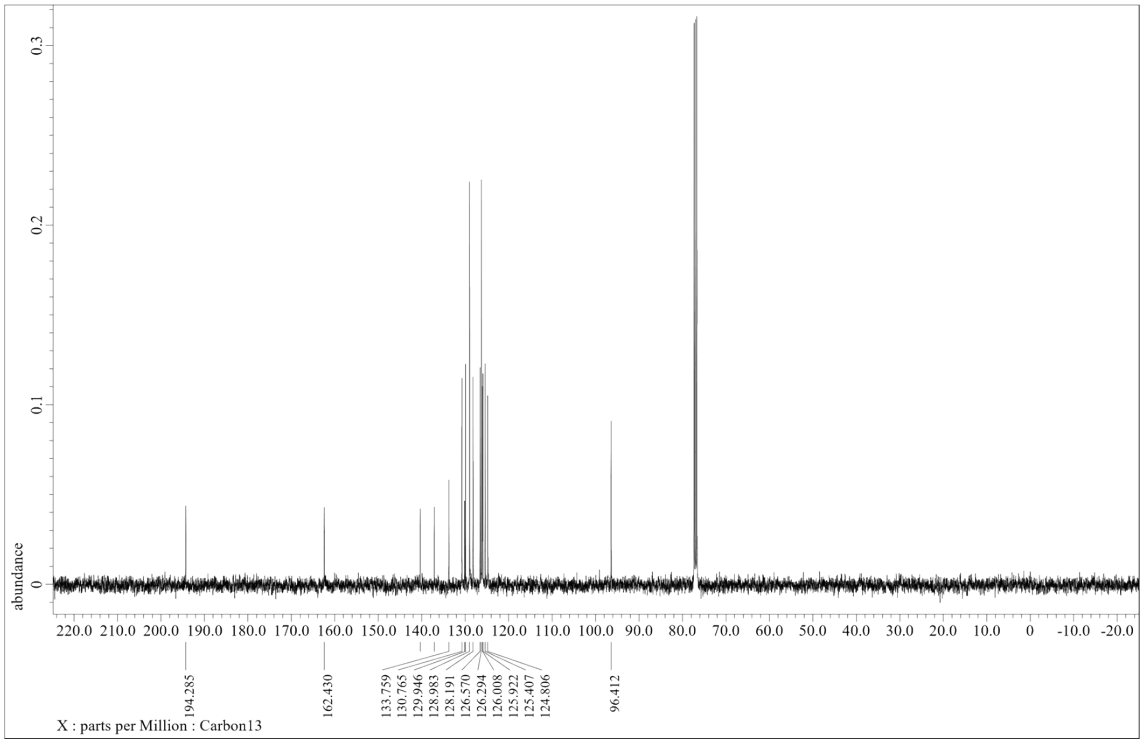
(*Z*)-3-amino-1-(naphthalen-1-yl)-3-phenylprop-2-en-1-one (11). Colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.60 (br, 1H), 5.95 (s, 1H), 7.40-7.54 (m, 6H), 7.60 (d, *J* = 6.9 Hz, 2H), 7.71 (d, *J* = 6. Hz, 1H), 7.87 (t, *J* = 8.2 Hz, 2H), 8.49 (d, *J* = 7.8 Hz, 1H), 10.46 (br, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 96.41, 124.81, 125.41, 125.92, 126.01, 126.29, 126.57, 128.98, 129.95, 130.14, 130.77, 133.76, 137.10, 140.34. IR (neat) 3457, 3342, 3176, 3061, 2924, 2846, 1603, 1567, 1523, 1484, 1402, 1312, 1231, 1183, 1132, 987, 912 cm^{-1}. HRMS (ESI) calcd. for $(M+Na)^+$ 296.1046, found 296.1046.

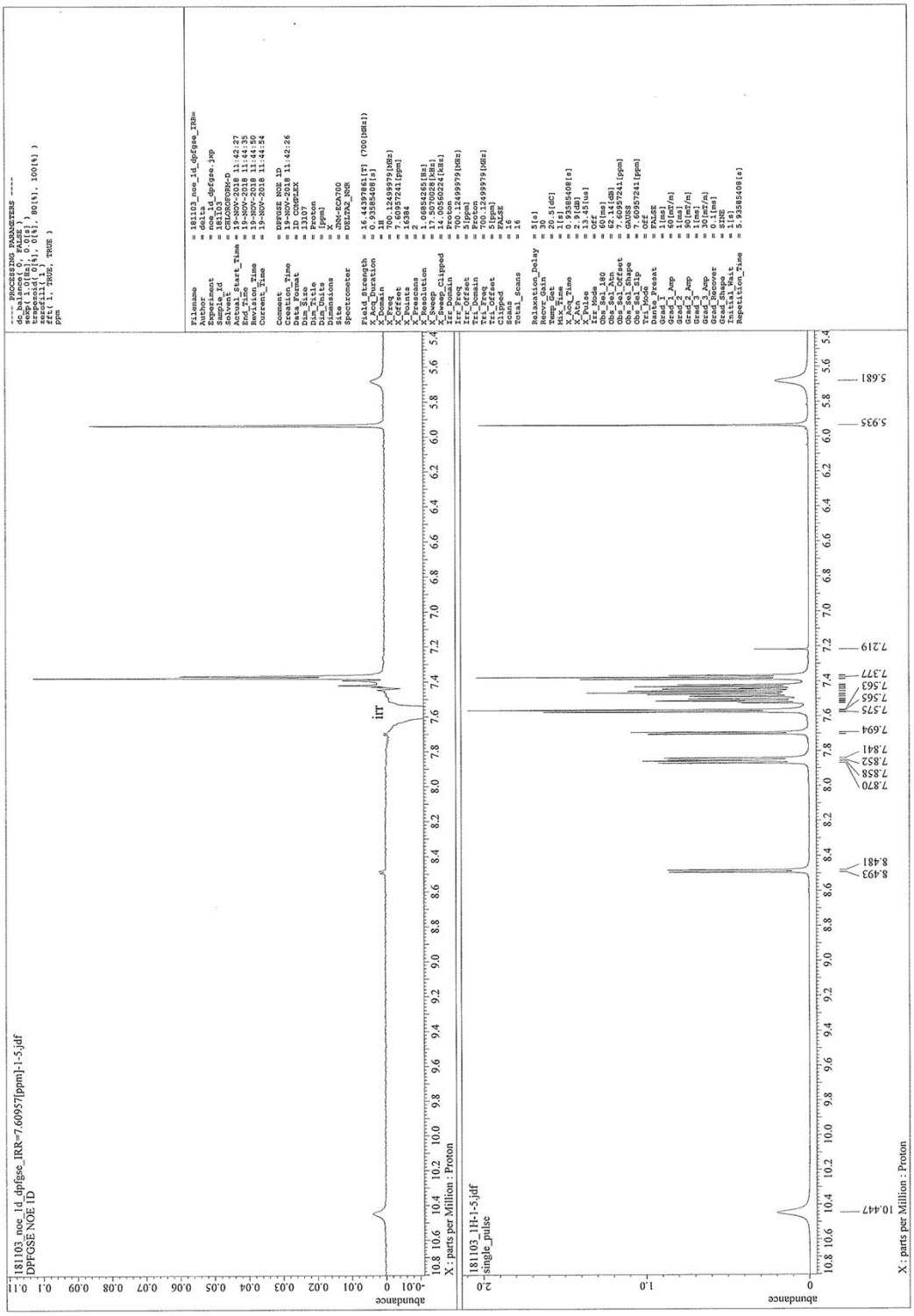
Representative NOE to determine the structure of **11** are shown in Figure S5.

Figure S5. Representative NOE of 11.

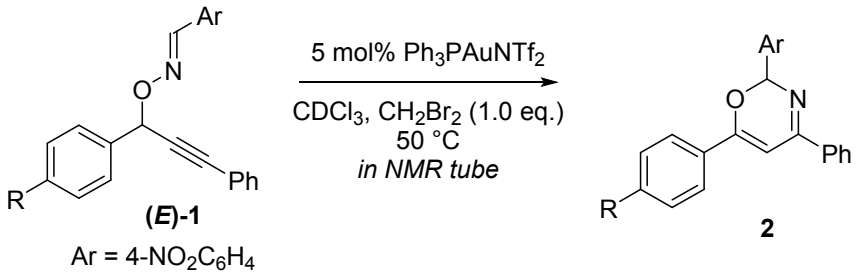



O
NH2
Ph
abundance
0.89
0.99
2.03
2.04
1.04
6.10
1.00
0.88
10.459
8.495
8.475
7.867
7.611
7.593
7.504
7.485
7.467
7.449
7.435
5.950
5.599
X : parts per Million : Proton


abundance
194.285
162.430
133.759
130.765
129.946
128.983
128.191
126.570
126.294
126.008
125.922
125.407
124.806
96.412
X : parts per Million : Carbon13


181103_noe_1d_dpfgse_IRR=7.60957[ppm]-1-5.jdf
DPFGSE NOE 1D
X : parts per Million : Proton
181103_1H-1-5.jdf
single_pulse
10.447
8.493
8.481
7.870
7.858
7.852
7.841
7.694
7.575
7.565
7.563
7.377
7.219
5.935
5.681

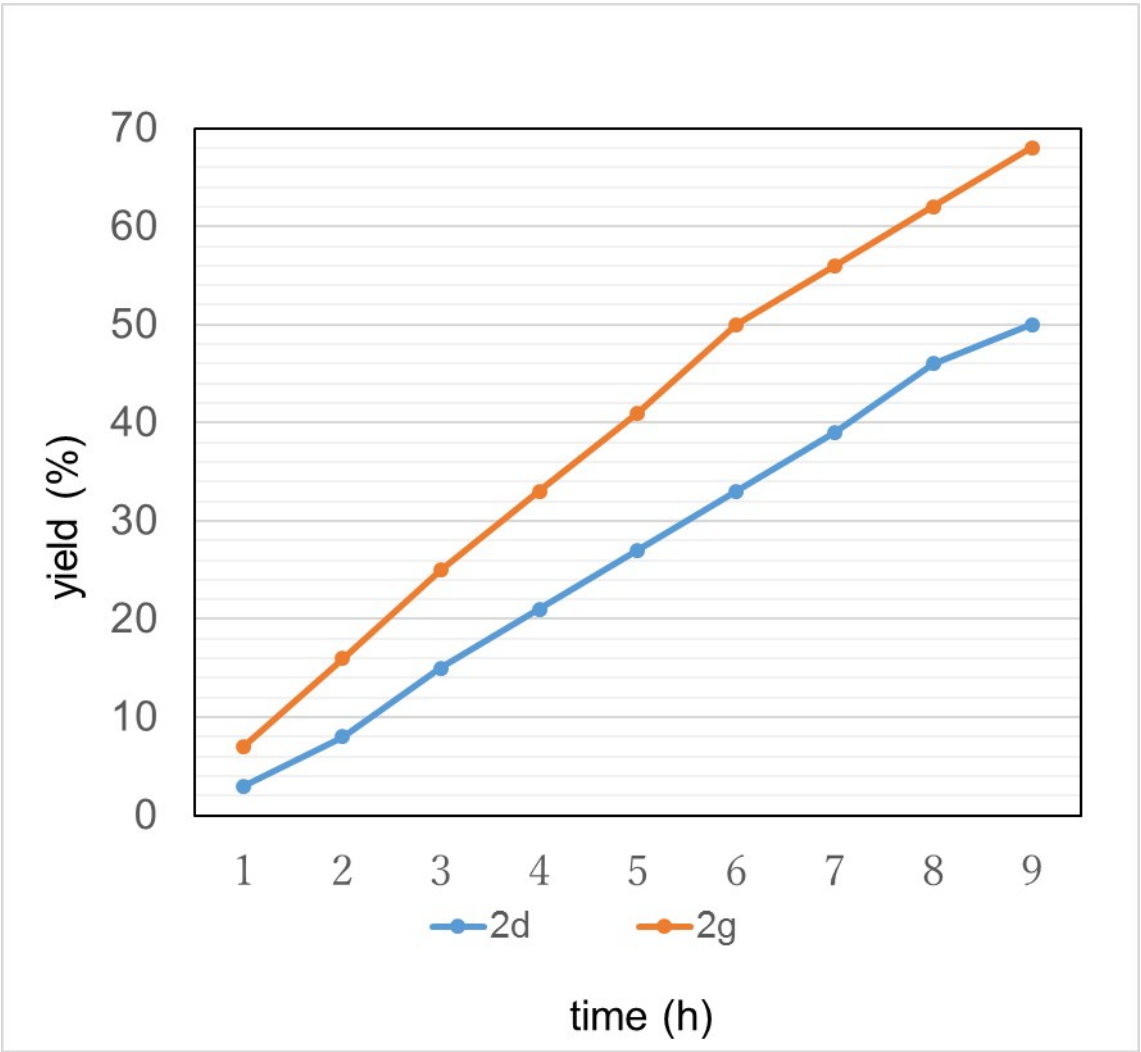
15. Appendix 2. Monitoring of Au-catalyzed reaction of 1d and 1g



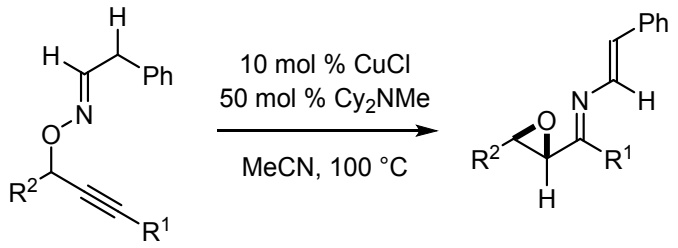
1d : R = H
1g : R = CF_3

2d : R = H
2g : R = CF_3

Figure S6. Progress of the Au-catalyzed reaction of **1d** and **1g**



16. Appendix 3. A plausible mechanism for the Cu-catalyzed rearrangement of *O*-propargylic oxime via N-O bond cleavage.



R^1, R^2 = aryl, alkyl

Nakamura, I.; Iwata, T.; Zhang, D.; Terada, M. *Org. Lett.* 2012, **14**, 206.

Scheme S2. Plausible mechanism for Cu-catalyzed rearrangement of *O*-propargylic oxime via N-O bond cleavage