Supporting Information

Thiocyanate Radical Mediated Dehydration of Aldoximes with Visible Light and Air

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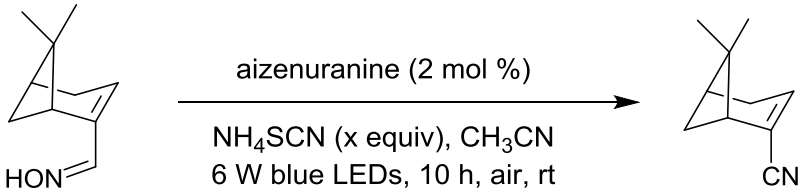
Content

I. General Procedures

^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker AM-400 MHz instruments in $CDCl_3$ with TMS as internal standard. The chemical shifts (δ) are reported in ppm and coupling constants (*J*) in Hz. Chemical shifts are reported in parts per million (δ) relative to $CDCl_3$ (7.27 ppm) for ^{1}H NMR data and $CDCl_3$ (77.0 ppm) for ^{13}C NMR data or the peak of DMSO-d_6, defined at δ = 2.50 (^{1}H NMR) or δ = 39.5 (^{13}C NMR). ^{19}F-NMR spectra were recorded on a BRUKER AVANCE III HD (376 MHz) spectrometer. Multiplicities are indicated, s (singlet), brs (broad singlet), d (doublet), t (triplet), q (quartet), dd (double doublets), m (multiplet). Mass spectra were obtained on BrukerESQ6K4. High resolution mass spectra and were performed on Bruker Daltonics APEXII 47e Specifications. Column chromatography was performed with silica gel (200-300 meshes). Thin layer chromatography (TLC) was visualized using UV light. GC-MS measurements were performed on a Thermo Scientific™ ISQ LT GC-MS instrument with Helium as the carrier gas. Emission spectroscopies were surveyed on a Perkin Elmer LS55 spectrofluorimeter. Ultraviolet-visible spectroscopy was performed on a Perkin Elmer Lambda 950 spectrophotometer. Cyclic voltammetry experiments were performed on a CH Instruments Electrochemical Analyzer. Materials were obtained from commercial suppliers or prepared according to standard procedures unless otherwise noted.

II. Detailed Reaction Optimizations

Table S1. Screen of the Molar Proportion of NH_4SCN and Sulfur Source for the Dehydration of Aldoximes[a]

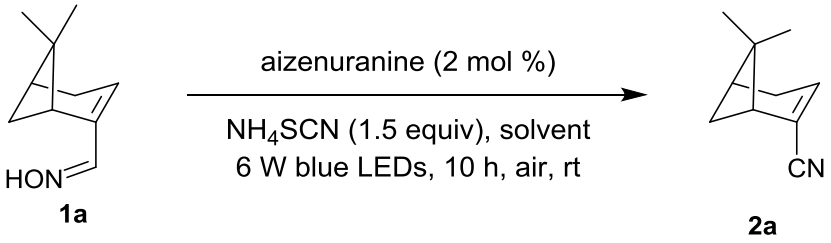


1a 2a

entry	NH_4SCN(x equiv)	yield (%)[b]
1	0	0
2	0.2	25
3	0.4	53
4	0.8	68
5	1.0	70
6	1.2	75
7	1.5	85
8	2.0	85
9	1.5 equiv NaSCN	76
10	1.5 equiv KSCN	74
11	1.5 equiv SDMP [c]	26
12	1.5 equiv potassium O-ethyl carbonodithioate	30
13	1.5 equiv potassium ethanethioate	0

[a] Reaction conditions: **1a** (0.2mmol, 1.0 equiv) and aizenuranine (0.002 mmol, 0.02 equiv) in 2.0 mL of dry CH_3CN under air with 6 W blue LED irradiation at rt for 10 h, unless otherwise noted. [b] Yields were determined by isolated yields. [c] SDMP: sodium 2,2-dimethylpropanethioate.

Table S2. Screen of Solvents for the Dehydration of Aldoximes[a]

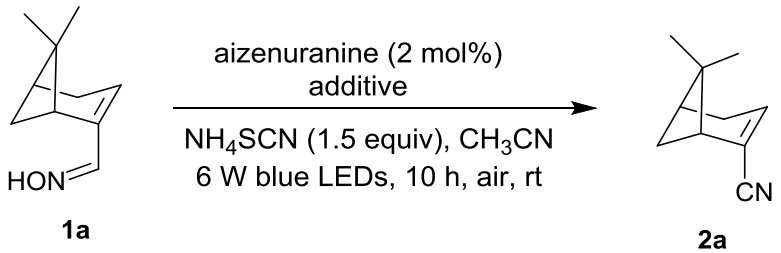


1a **2a**

entry	solvent	yield (%)[b]
1	acetone	61
2	DCE	22
3	EtOH	12
4	1,4-dioxane	27
5	THF	32
6	MeOH	17
7	$CH_3CN:H_20$ = 10:1	39

[a] Reaction conditions: **1a** (0.2 mmol,1.0 equiv), NH_4SCN (0.3 mmol,1.5 equiv) and aizenuranine (0.002 mmol, 0.02 equiv) in 2.0 mL of dry solvent under air with 6 W blue LED irradiation at rt for 10 h, unless otherwise noted .[b] Yields were determined by isolated yields.

Table S3. Screen of Additives for the Dehydration of Aldoximes[a]

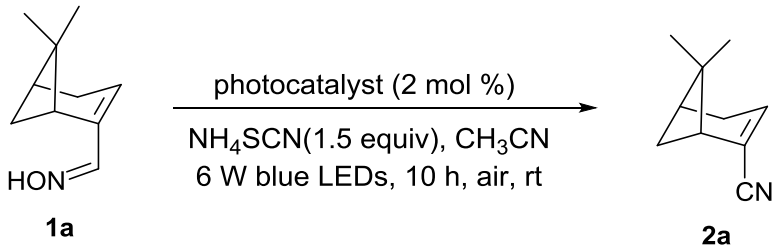


1a **2a**

entry	additive	yield (%)[b]
1	15 mg 4Å	79
2	50 mg 4Å	72
3	2.0 equiv AcOH	69
4	2.0 equiv K_2CO_3	17
5	2.0 equiv K_2HPO_4	26
6	2.0 equiv KH_2PO_4	63

[a] Reaction conditions: **1a** (0.2mmol, 1.0 equiv) , NH_4SCN (0.3 mmol, 1.5 equiv) and aizenuranine (0.002 mmol, 0.02 equiv) in 2.0 mL of dry CH_3CN under air with 6 W blue LED irradiation at rt for 10 h, unless otherwise noted. [b] Yields were determined by isolated yields.

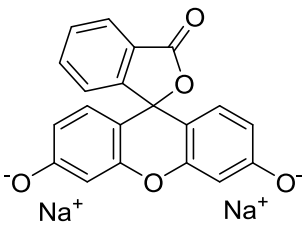
Table S4. Screen of Photocatalyst for the Dehydration of Aldoximes[a]



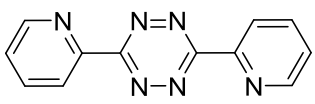
1a **2a**

entry	photocatalyst	yield (%)[b]
1	eosin Y	80
2	eosin B	62
3	fluorescein	51
4	aizenuranine	84
5	tetraiodofluorescein	61
6	Acr-Mes$^+$	46
7	rose bengal	68
8	2,4,6,-phenylpyrylium tertfluorborate	72
9	eosin Y-Na_2	72
10	basic red 1	54
11	$Ru(bpy)_3Cl_2$	67
12	TBAB-eosin Y	77
13	FIrPic	47
14	bptz[c]	63
15	$Ir(ppy)_3$	63
16	$Ir[dF((CF_3)ppy)_2(dtppy)]PF_6$	36
17	4CzIPN[d]	67

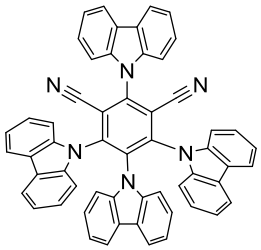
[a] Reaction conditions: **1a** (0.2 mmol, 1.0 equiv) , NH_4SCN (0.3 mmol,1.5 equiv) and photocatalyst (0.002 mmol, 0.02 equiv) in 2.0 mL of dry CH_3CN under air with 6 W blue LED irradiation at rt for 10 h, unless otherwise noted. [b] Yields were determined by isolated yields. [c] bptz: 3,6-Bis(2-pyridinyl)-1,2,4,5-tetrazine. [d] 4CzIPN :(4r,6r)-2,4,5,6-tetra(9H-carbazol-9-yl)-isophthalonitrile.



aizenuranine

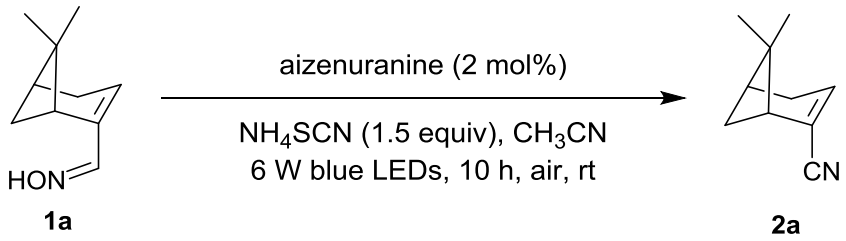


bptz



4CzIPN

Table S5. Control Experiments for the Dehydration of Aldoximes[a]

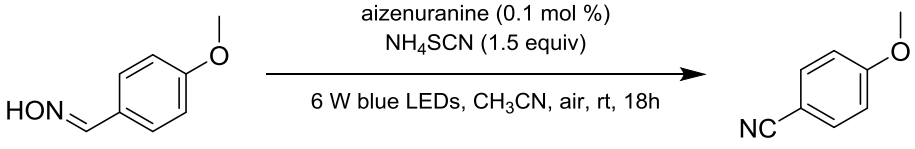


1a **2a**

Entry	Conditions	Yield (%)[b]
1	no light	0
2	no aizenuranine	0
3	no air	0

[a] Reaction conditions: **1a** (0.2 mmol, 1.0 equiv) , NH_4SCN (0.3 mmol,1.5 equiv) and aizenuranine (0.002 mmol, 0.02 equiv) in 2.0 mL of dry CH_3CN under air with 6 W blue LED irradiation at rt for 10 h, unless otherwise noted. [b] Yields were determined by isolated yields.

III. Gram-Scale for the Dehydration of 3e



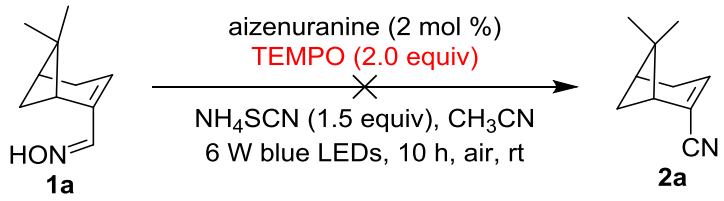
3e, 1.51g, 10 mmol

4e, 1.17g, 88%

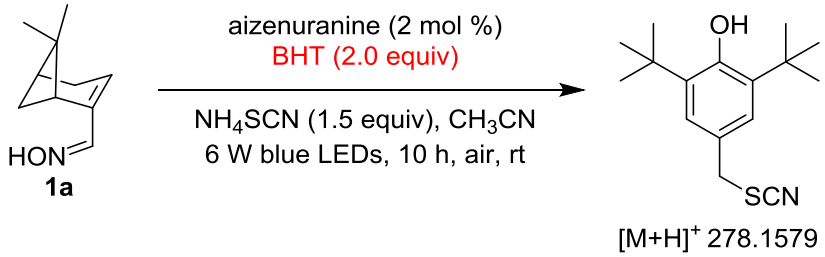
A 100 mL pyrex glass tube and was stirred with a Teflon-coated magnetic stir bar. Ammonium thiocyanate (15 mmol, 1.5 equiv) and aizenuranine (0.1 mol %) were added to the solution of **3e** (10 mmol, 1 equiv) in MeCN (40 mL). The reaction mixture was stirred at rt in the air and irradiated by 6 W blue LEDs. The reaction was monitored by TLC, after 18 hours, the solvent was removed under reduced pressure by rotary evaporator. Then, the crude residue was purified by recrystallization in the mixture of petroleum ether and ethyl acetate.

IV. Mechanistic Studies

The Radical Trapping Experiments



To a 10 mL pyrex glass tube which equipped with a magnetic stirring bar were added **1a** (1.0 equiv 0.2 mmol), aizenuranine (2 mol %) and NH_4SCN (1.5 equiv, 0.3 mmol) followed by TEMPO (2.0 equiv) in dry CH_3CN (2 mL). The reaction mixture was stirred at rt in the air and irradiated by 6W blue LEDs for 10 hours. The reaction was monitored by TLC. No desired product **2a** was observed and starting material was recovered.



To a 10 mL pyrex glass tube which equipped with a magnetic stirring bar were added **1a** (1.0 equiv, 0.2 mmol), aizenuranine (2 mol %) and NH_4SCN (1.5 equiv, 0.3mmol) followed by BHT (2.0 equiv) in dry CH_3CN (2 mL). The reaction mixture was stirred at rt in the air and irradiated by 6 W blue LEDs for 10 hours. The reaction was monitored by TLC and was characterized by high resolution mass spectra. (Related literatures: (a) Tong, K.; Liu, X. D.; Zhang, Y.; Yu, S. Y.; *Chem. Eur. J.* **2016**, *22*, 15669. (b) Egami, H.; Ide, T.; Kawato, Y.; Hamashima, Y.; *Chem. Commun.* **2015**, *51*, 16675. (c) Gao, Y. Z.; Lu, G. Z.; Zhang, P. B.; Zhang, L. L.; Tang, G.; Zhao, Y. F. *Org. Lett* .**2016**, *18*, 1242.)

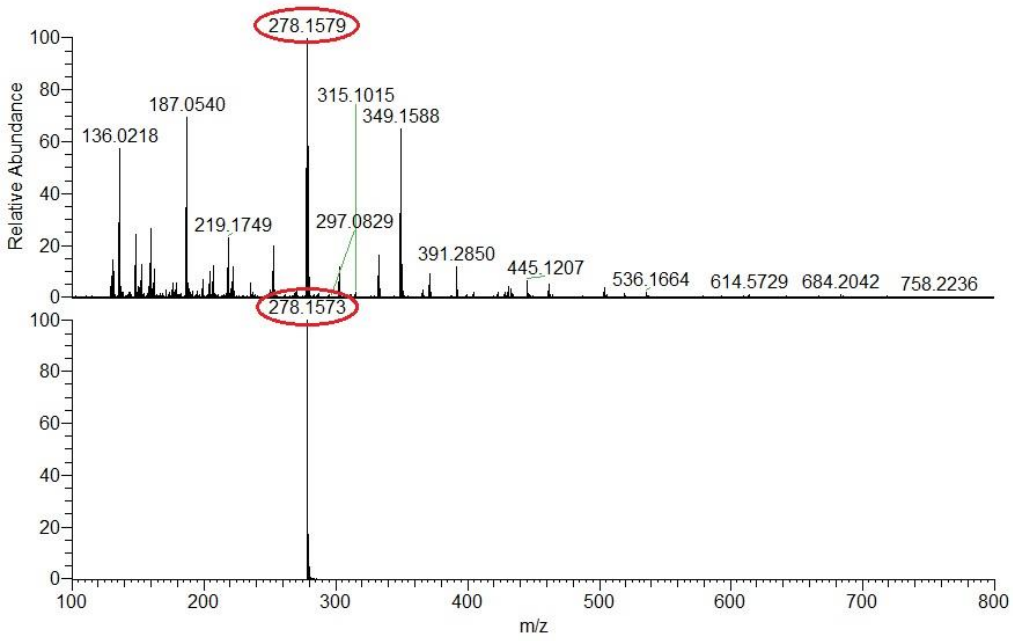
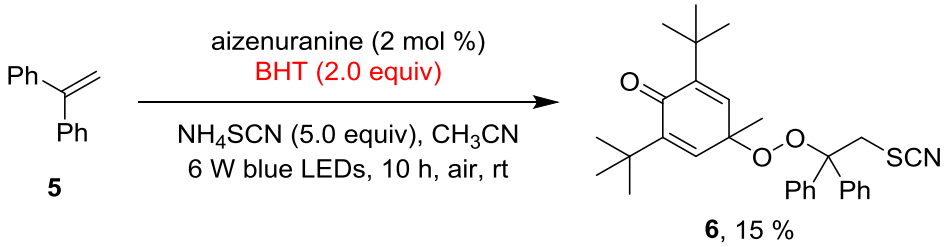


Figure S1. ESI-HRMS of the BHT-SCN



To a 10 mL pyrex glass tube which equipped with a magnetic stirring bar were added 1,1-diphenylethylene (**5**, 1.0 equiv 0.2 mmol), BHT (2.0 equiv) aizenuranine (2 mol %) and NH_4SCN (5 equiv, 1.0 mmol) in dry CH_3CN (2 mL). The reaction mixture was stirred at rt in the air and irradiated by 6 W blue LEDs for 10 hours. The reaction was monitored by TLC. The solvent was removed under reduced pressure by rotary evaporator. Then, the residue was purified by silica gel column chromatography to give the corresponding product **6**.

2,6-di-*tert*-butyl-4-((1,1-diphenyl-2-thiocyanatoethyl)peroxy)-4-methylcyclohexa-2,5-dien-1-one (6): yellow liquid, 14.2 mg, (Yield: 15 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.30 (dd, *J* = 6.0 Hz, 6H), 7.19 (m, 4H), 6.50 (s, 2H), 4.21 (s, 2H), 1.27 (s, 21H); **^{13}C NMR** (100 MHz, $CDCl_3$)**:** δ 186.3, 141.1, 140.9, 128.4, 128.2, 126.4, 113.0, 85.3, 77.7, 42.6, 34.8, 29.5, 23.6; **HRMS (ESI)** for Chemical Formula: $C_{11}H_{14}NO$

$(M+H)^+$ Calcd: 490.2407, Found: 490.2410.

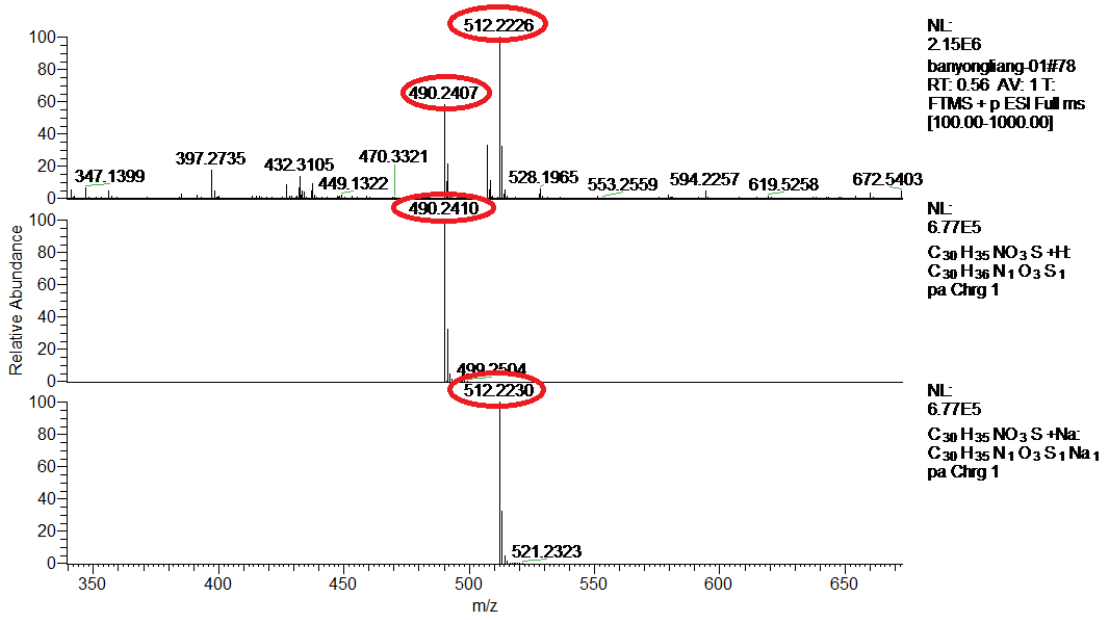
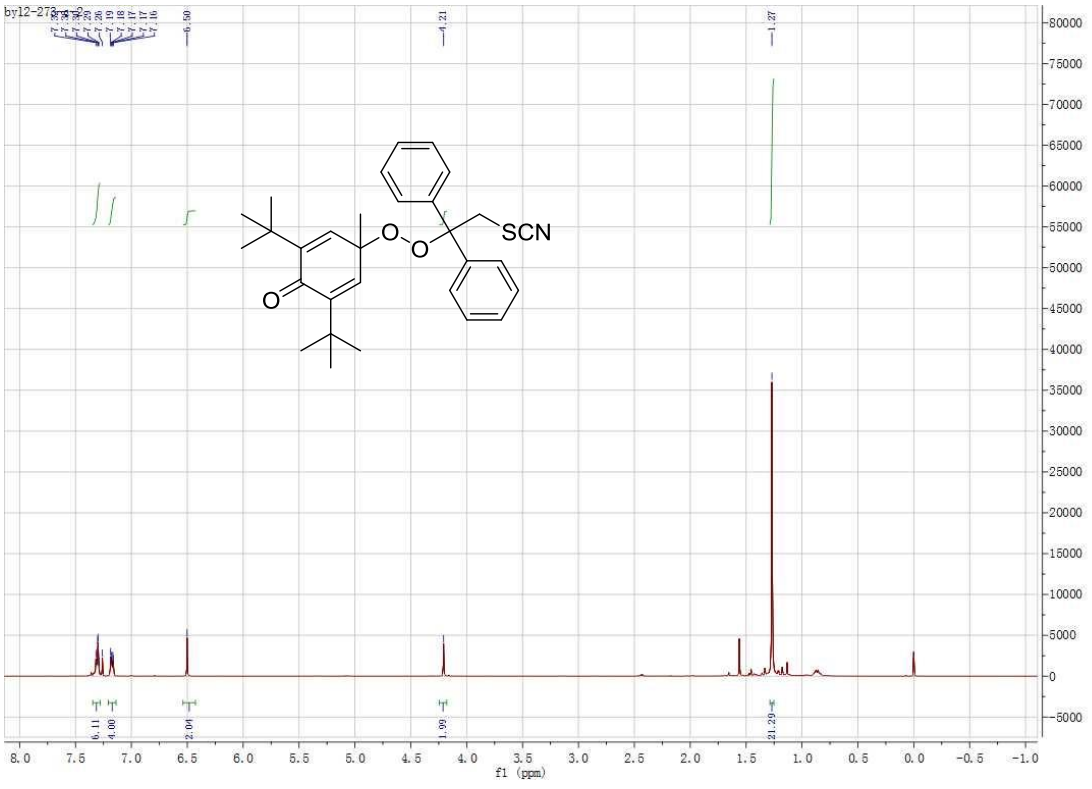
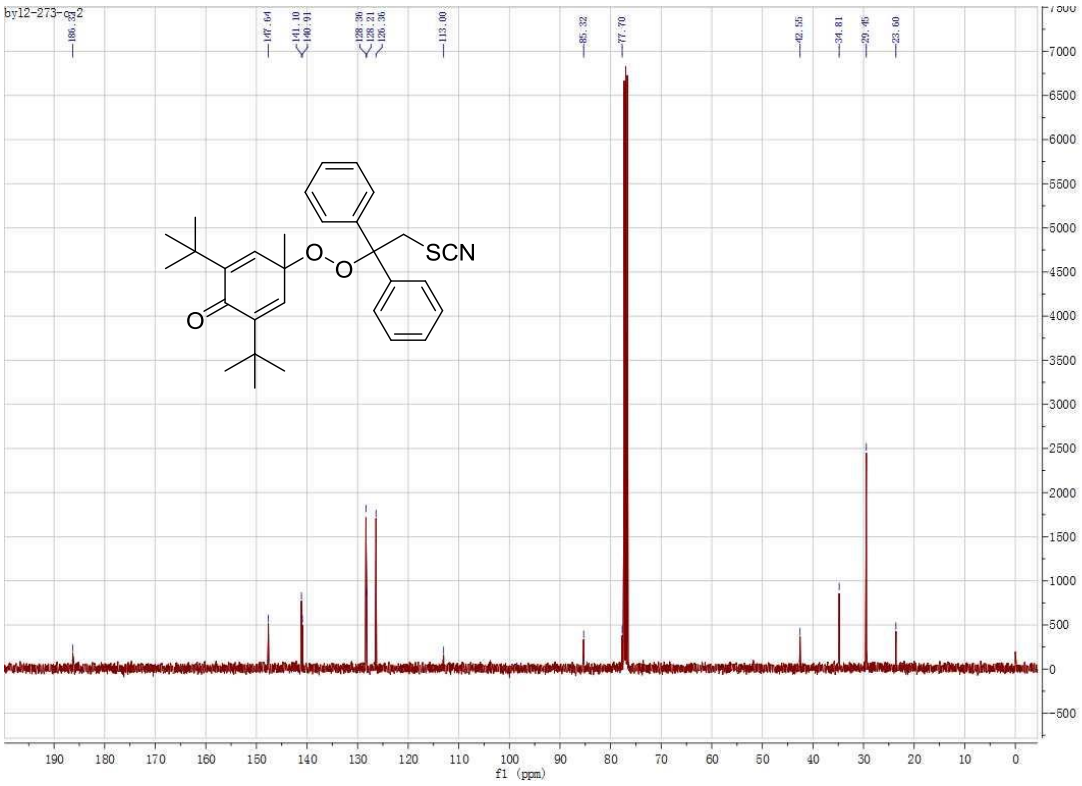


Figure S2. ESI-HRMS of 6





Excitation and Emission Spectra of Aizenuranine

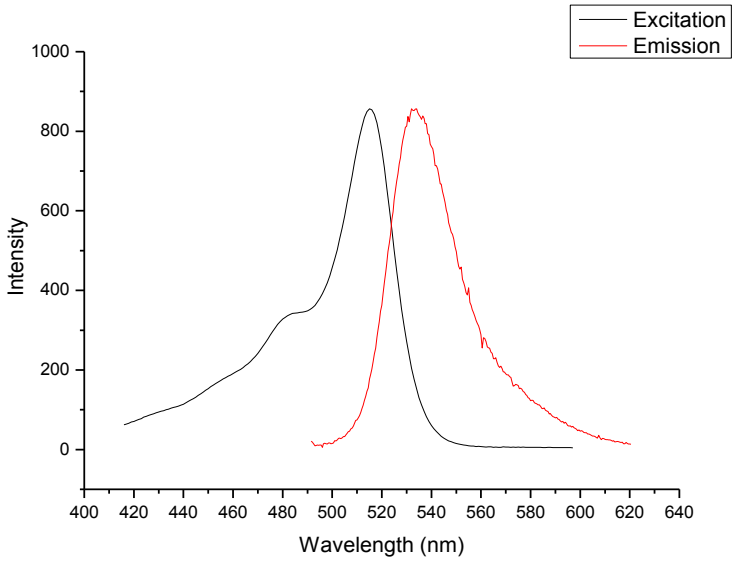


Figure S3. Excitation and Emission Spectra of Aizenuranine.

The Cyclic Voltammetry Experiments

Cyclic voltammetry experiments were performed on a CH Instruments Electrochemical Analyzer at room temperature under a nitrogen atmosphere. The 1 mM CH_3CN solution of **1a** was prepared with 100 mM tetrabutylammonium tetrafluoroborate as the supporting electrolyte, using a glassy carbon working electrode, a Pt counter electrode, and a $Hg/HgCl_2$ reference electrode. Scan Rate (V/s) = 0.05.

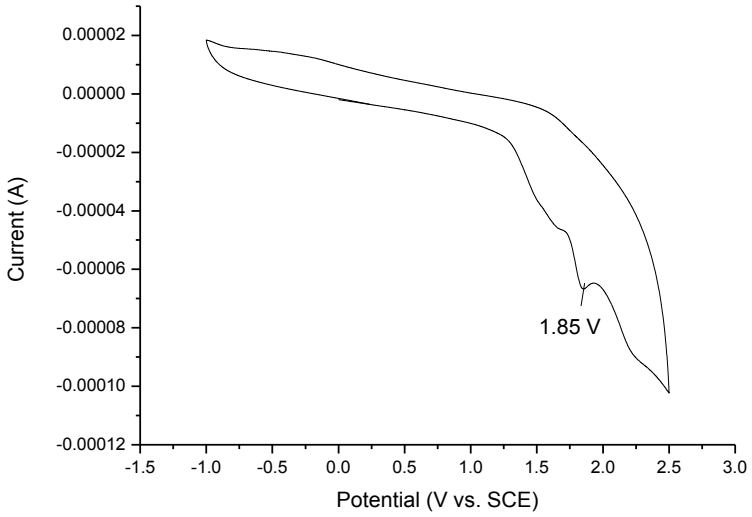


Figure S4. The Cyclic Voltammetry Experiment of 1a

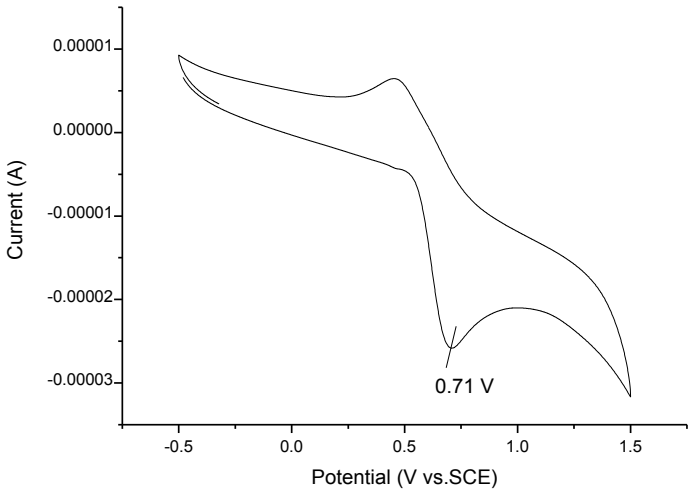


Figure S5. The Cyclic Voltammetry Experiment of NH_4SCN

aizenuranine[1] (PC): $PC/PC^{\bullet-}$ $E_{P/2} = -1.22$ V vs. SCE

$PC^{\bullet-}/PC$ $E_{P/2} = +0.83$ V vs. SCE

The reduction potential of excited aizenuranine is estimated from Gibbs energy of photoinduced electron transfer using the ground state potentials[2] and the energy gap between zero vibrational levels of the ground and excited states ($E_{0,0}$). The latter value is approximated as the wavelength at which excitation and emission intersection.

$$E(PC^*/PC^{\bullet-}) = E\,(PC/PC^{\bullet-}) + E_{0,0}$$

$$= -1.22\text{ V} + 2.37\text{ V}$$

$$= +1.15\text{ V vs. SCE}$$

Identifying the Formation of Thiocyanogen by GC-MS

To a 10 mL pyrex glass tube which equipped with a magnetic stirring bar were added **3e** (1.0 equiv, 0.2 mmol), aizenuranine (2 mol %) and NH_4SCN (1.5 equiv, 0.3 mmol) in dry CH_3CN (2 mL). The reaction mixture was stirred at rt in the air and irradiated by 6 W blue LEDs. After stirring for 4 hours, the mixture was analyzed by GC-MS.

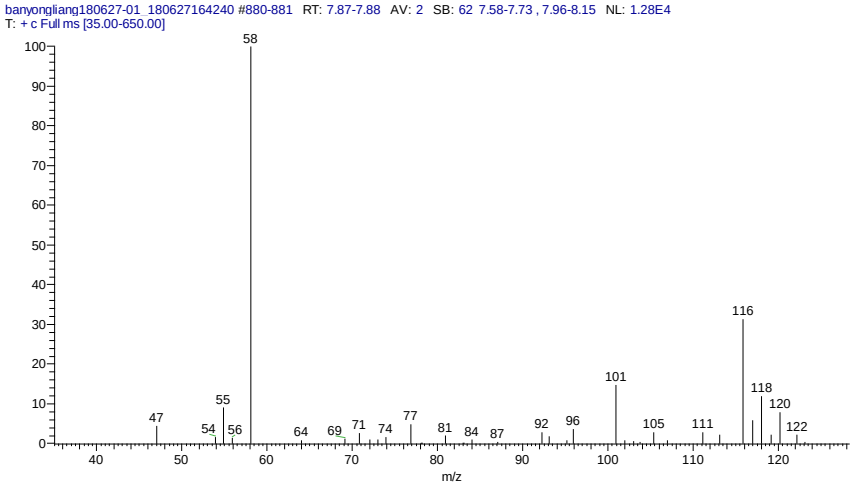


Figure S6. GC-MS Spectra of the Mixture, the m/z=116 was found.

Theoretical Calculations

Calculation method

Quantum mechanical calculations were performed using Gaussian 09[1]. All geometries and single point energies were calculated with M06-2x/6-31+G(d,p) and SMD solvation model for acetonitrile[2]. The vibrational frequencies at the same level were computed to characterize all optimized structure as minima or a transition state and to evaluate its zero-point vibrational energy (ZPVE) and thermal corrections at 298 K.

Coordinates of all stationary points

Table S6. Sum of electronic and thermal free energies (G, in a.u.), sum of electronic and thermal enthalpies (H, in a.u.), Sum of electronic and zero-point energies (E, in a.u.), and imaginary frequencies for the transition states (IF).

structure	*G*	*H*	*E*	*IF*
$^{\cdot}$SCN	-490.928521	-490.902160	-490.906417	
HSCN	-491.558351	-491.528999	-491.533604	
$(SCN)_2$	-981.908145	-981.869128	-981.876694	
$O_2^{\bullet-}$	-150.401021	-150.377944	-150.381260	
$HO_2^{\cdot}$	-150.864487	-150.838540	-150.842334	
$NCSO^-$	-566.272520	-566.240382	-566.245499	
3a	-400.640991	-400.600031	-400.608398	
TS1	-891.550407	-891.496341	-891.508716	-561.1
INT1	-400.015111	-399.974360	-399.982446	
TS2	-890.913973	-890.862222	-890.874177	-257.2
INT2	-890.971292	-890.919539	-890.931324	
TS3	-1041.354151	-1041.354151	-1041.309360	-875.5
4a	-324.312886	-324.275557	-324.282598	
TS1b	-1382.451048	-1382.390478	-1382.406416	-316.0
INT1b	-1382.514942	-1382.450982	-1382.467937	

Coordinates for the ground states an transition states involved

$^{\cdot}$SCN

S	-0.01891800	-1.02219600	0.00000000
C	0.00000000	0.62802800	0.00000000
N	0.04324100	1.79814000	0.00000000

HSCN

S	2.13681500	0.22765200	0.00000000
H	3.47712700	0.07192600	0.00000000
C	2.21341600	1.92879900	0.00000000
N	2.20160000	3.08775700	0.00000000

$(SCN)_2$

S	-0.91435000	-0.12699200	-0.00336200
S	-2.41833800	1.32902400	-0.00336200
C	-1.83906300	2.34367000	1.23996100
C	-1.49362500	-1.14163800	1.23996100
N	-1.49353600	3.06386100	2.07927600
N	-1.83915300	-1.86182900	2.07927600

$O_2^{\bullet-}$

O	0.00000000	0.00000000	0.66219800
O	0.00000000	0.00000000	-0.66219800

$HO_2^{\bullet}$

O	0.33380800	0.10346600	0.00000000
O	-0.96714200	-0.04681600	0.00000000
H	-1.35247900	0.85748000	0.00001800

$NCSO^-$

O	-2.27298200	-0.25954500	0.00000000
S	-1.39778000	-1.57503100	0.00000700
C	0.24929700	-1.06710300	0.00000300
N	1.36814000	-0.73096200	0.00000100

3a

C	0.47539300	-0.06279700	-0.00626000
C	-0.57743100	-0.97745900	-0.00623000
C	-0.30390600	-2.34602100	-0.00621800
C	1.01491800	-2.78759400	-0.00623600
C	2.08598100	-1.87651400	-0.00626600
C	1.79953500	-0.49913900	-0.00627800
H	0.26784200	1.00320100	-0.00626900
H	-1.60496600	-0.62596200	-0.00621600
H	-1.11605700	-3.06681400	-0.00619400
H	1.22632800	-3.85397400	-0.00622600
H	2.60043700	0.22655500	-0.00630200
C	3.42981600	-2.48352100	-0.00628000
H	3.45088900	-3.57220100	-0.00625300
N	4.60534300	-1.97779700	-0.00631900
O	4.62545700	-0.59350200	-0.00635500
H	5.56975400	-0.37517200	-0.00637800

TS1

C	-1.39210400	0.36082000	-0.00812000
C	-2.20920100	-0.77095400	-0.07865700

C	-1.71347100	-2.02776100	0.27523400
C	-0.39895700	-2.15434900	0.70391900
C	0.41890500	-1.01330400	0.80021300
C	-0.07627500	0.24761000	0.42223700
H	-1.77937500	1.33079000	-0.30149800
H	-3.23448300	-0.67305900	-0.42229100
H	-2.34970200	-2.90441900	0.21373600
H	0.00267100	-3.12416700	0.98266100
H	0.55730800	1.12759200	0.44476500
C	1.75678400	-1.23188300	1.32103600
H	2.09954800	-2.24905800	1.49885500
N	2.65125500	-0.32866400	1.52148400
O	2.47657600	0.92372700	1.68052900
H	3.31999300	1.47699000	1.09954800
S	4.56932200	2.19954400	0.21882500
C	5.06203800	0.73984700	-0.46163600
N	5.41614600	-0.26263900	-0.94174100

INT1

C	1.30118200	-0.46715400	-0.00012300
C	0.22830200	-1.35880100	-0.00011900
C	0.46771500	-2.73451600	-0.00011800
C	1.77357800	-3.21383500	-0.00011800
C	2.85628200	-2.32098000	-0.00012400
C	2.61217800	-0.94015900	-0.00012700
H	1.11907500	0.60324100	-0.00012200
H	-0.79064500	-0.98362300	-0.00011700
H	-0.36351800	-3.43312800	-0.00011500
H	1.96622300	-4.28349100	-0.00011600
H	3.43647000	-0.23425900	-0.00013000
C	4.20680100	-2.90067700	-0.00012600
H	4.32907900	-3.97843100	-0.00008700
N	5.29478000	-2.22417600	-0.00016800
O	5.55738700	-1.02182200	-0.00022400

TS2

C	-1.72093400	1.39922200	-0.01145400
C	-0.43242600	0.86735900	-0.09657200
C	-0.22232900	-0.36982500	-0.70658100
C	-1.29874400	-1.07873400	-1.23291000
C	-2.58875100	-0.54239800	-1.14606900
C	-2.80278800	0.69747100	-0.53459900
H	-1.88341600	2.36206100	0.46237400
H	0.40827700	1.41905100	0.31325200

H	0.77905000	-0.78337400	-0.77442100
H	-1.14798400	-2.04281400	-1.71048200
H	-3.80175500	1.12093600	-0.46258400
C	-3.69261400	-1.33066100	-1.72743900
H	-3.49633900	-2.28637300	-2.20850500
N	-4.89508800	-0.94306400	-1.69708600
O	-5.69301300	-0.10482400	-1.37928000
S	-7.87833700	-0.49859100	-1.96176100
C	-8.24759200	0.85025400	-1.05750800
N	-8.45404400	1.80231600	-0.41295200

INT2

C	-2.03297400	-0.12927600	-0.08274300
C	-0.79927600	-0.76274100	0.07051400
C	-0.74389300	-2.14877700	0.21741000
C	-1.91997000	-2.89130200	0.21084200
C	-3.16774900	-2.26552400	0.04624200
C	-3.21393500	-0.86719000	-0.09913700
H	-2.07931300	0.94995100	-0.19149200
H	0.11503100	-0.17696900	0.07828500
H	0.21119200	-2.64959600	0.34125700
H	-1.87910400	-3.97047200	0.33239400
H	-4.15752200	-0.35252400	-0.21648600
C	-4.32682200	-3.17263300	0.05960800
H	-4.11080000	-4.21082700	0.31226600
N	-5.57314600	-3.01425600	-0.18065100
O	-5.88098700	-1.67003300	-0.52649500
S	-7.48410300	-1.50939900	-0.91220900
C	-8.13286500	-1.39435400	0.66614500
N	-8.60424500	-1.31440500	1.72277800

TS3

C	-0.95378000	0.11471000	0.15749700
C	-2.22951200	0.43252700	-0.31557700
C	-2.39937600	1.52058300	-1.17109600
C	-1.30078700	2.29477300	-1.54524900
C	-0.01670100	1.96102000	-1.09813000
C	0.14964800	0.86805100	-0.23499200
H	-0.81770400	-0.72612800	0.83162700
H	-3.08676400	-0.16136500	-0.01257900
H	-3.38925400	1.77886600	-1.53592800
H	-1.43512200	3.15910300	-2.19080200
H	1.14285700	0.61661700	0.12553300
C	1.12039900	2.83141200	-1.46492500

H	0.97978900	4.22371000	-1.30074000
N	2.24132500	2.52300100	-1.92481400
O	2.33295300	0.92327200	-2.20642700
S	3.87949500	0.44276600	-2.14656800
C	4.09962200	0.27839100	-0.45188200
N	4.25663900	0.16693500	0.69384900
O	0.78064000	5.38173000	-1.05725300
O	0.44499400	5.37332600	0.20891900

4a

C	-1.41516800	-0.45193200	0.00593000
C	-0.72203300	-1.66356300	0.00593100
C	-1.41516800	-2.87519300	0.00593100
C	-2.80651400	-2.88340500	0.00593000
C	-3.49503400	-1.66356300	0.00592900
C	-2.80651400	-0.44372000	0.00592900
H	-0.87189200	0.48750900	0.00593000
H	0.36377900	-1.66356300	0.00593200
H	-0.87189300	-3.81463500	0.00593200
H	-3.35976700	-3.81697000	0.00593000
H	-3.35976700	0.48984500	0.00592800
C	-4.93454800	-1.66356200	0.00592800
N	-6.09291900	-1.66356200	0.00592700

TS1b

C	0.12999300	-0.10865100	-0.09611900
C	-1.10985000	-0.18320200	0.54211900
C	-1.75903500	0.98218500	0.95524400
C	-1.16579900	2.21912000	0.73277000
C	0.10130000	2.29902200	0.12843200
C	0.74175500	1.12267300	-0.30132500
H	0.62693200	-1.01364500	-0.43239700
H	-1.57603300	-1.15023400	0.70593400
H	-2.72921000	0.92504900	1.43834900
H	-1.66990100	3.13259300	1.03648000
H	1.69666600	1.16341700	-0.81232100
C	0.64502600	3.64590900	-0.05372400
H	-0.06971200	4.46497400	-0.13242600
N	1.85866900	4.07277800	-0.11081900
O	2.78397800	3.02500300	0.06355400
S	3.05388900	2.50553600	2.11764300
C	2.85872600	0.85890000	2.19997000
N	2.71181100	-0.29854000	2.24686800
H	3.66813500	3.38473100	-0.18403300

S	5.31805400	1.54939300	0.26281400
C	4.40446600	0.29115300	-0.32144200
N	3.73288000	-0.59837000	-0.68202800

INT1b

C	3.53974900	0.11740800	0.00867400
C	2.31356300	-0.12989200	0.62809700
C	1.65474100	0.89539000	1.30819100
C	2.22795500	2.16178700	1.37659300
C	3.48010100	2.40383600	0.79272200
C	4.12642000	1.37688800	0.09107700
H	4.04545300	-0.67347300	-0.53681600
H	1.86662200	-1.11773900	0.57031300
H	0.69430700	0.71086300	1.77902100
H	1.71665100	2.96657600	1.89803700
H	5.06853900	1.56578800	-0.40759800
C	4.03051900	3.75704300	0.98209200
H	3.31206500	4.57415600	1.06433700
N	5.23008400	4.17080800	1.14479300
O	6.18418000	3.08821500	1.03967600
S	7.00131000	2.88547500	2.46954900
C	5.89368600	1.83344000	3.24297800
N	5.14927000	1.12197300	3.77691700
H	7.50112000	2.31466500	-0.62461500
S	8.30130800	1.24302500	-0.81741800
C	7.46278000	0.27243700	0.30172300
N	6.92603500	-0.42929000	1.05293200

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2. Y. Zhao, D. G. Truhlar, The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited

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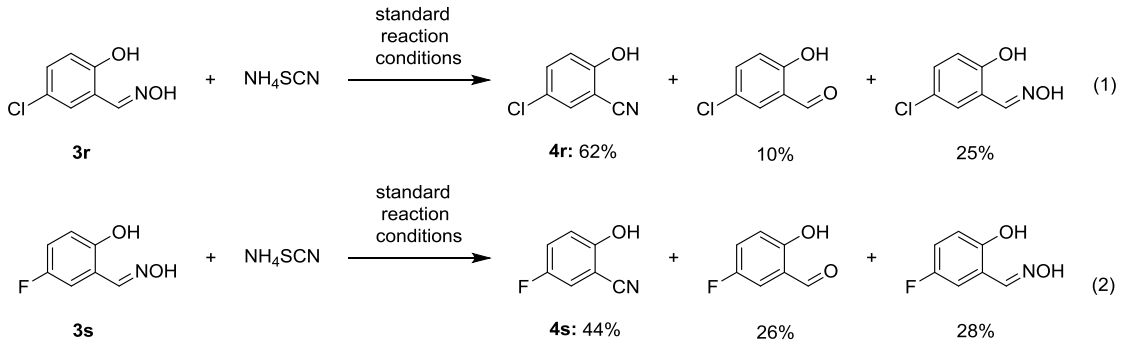
By-products Separation

According to the suggestion of the referee, the by-products of aldoximes **3r** and **3s** in the standard conditions were identified. In the case of **3r**, 62% of **4r** and 10% of by-product aldehyde were isolated at 75% conversion; In the case of **3s**, 44% of **4s** and 26% of by-product aldehyde were isolated at 72% conversion. According to a recent report, the oxidative deoximation reaction might occur with air oxidant (*Adv. Synth. Catal.*, 2019, 361, 603).



General procedure of the ESR experiments

ESR spectra were recorded at 300K using a Bruker A300 EPR spectrometer at 9.4453 GHz, The calculated g values are obtained by using 2,2-diphenyl-1-picrylhydrazyl (DPPH) as a standard. The EPR parameters were set as the following: sweep width 120 G, center field 3364 G, time constant 81.92 ms, sweep time 60.00 s, microwave power 25.10 mW, modulation amplitude 1.00 G, modulation frequency 100 kHz, and receiver gain 2.00×10^4.

a: To a 10 mL pyrex glass tube which equipped with a magnetic stirring bar were added aizenuranine (2 mol %), NH_4SCN (1.0 equiv, 0.60 mmol) in dry CH_3CN (1 mL). The reaction mixture was stirred at rt in the air and irradiated by 6 W blue LEDs for 0.5h. The EPR spectrum is shown in Figure S7 a.

b: To a 10 mL pyrex glass tube which equipped with a magnetic stirring bar were added aizenuranine (2 mol %), NH_4SCN (1.0 equiv, 0.60 mmol) in dry CH_3CN (1 mL). The reaction mixture was stirred at rt in the air and irradiated by 6 W blue LEDs for 0.5h. Subsequently, 5,5-dimethyl-1-pyrroline-*N*oxide (DMPO) (0.90 mmol, 1.5 equiv) wadded and stirred 1min. The EPR spectrum is shown in Figure S7 b. Data analysis suggests that an in situ generated thiocyanate radical is promptly trapped by DMPO to produce the metastable radical **(**α_N = 14.42 G, α_H = 16.82 G, and g = 2.0054**),** which is consistent with the previous report (*J. Biol. Chem.* **1997**, *272*, 11049.). The example for ESR detection was also detected by HRMS and the results is shown in Figure S8.

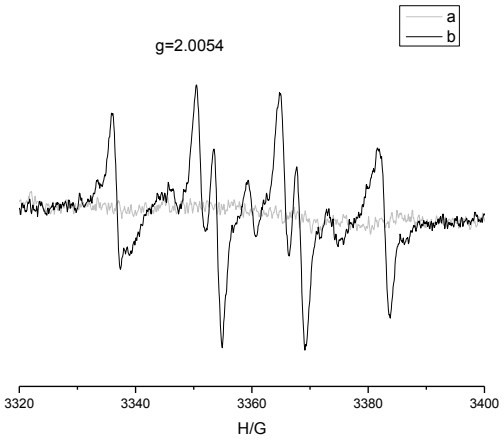


Figure S7. ESR measurements of (a) a CH_3CN solution of aizenuranine and NH_4SCN under the irradiation of 6W blue LEDs; (b) a CH_3CN solution of aizenuranine and NH_4SCN in the presence of DMPO under the irradiation of 6W blue LEDs.

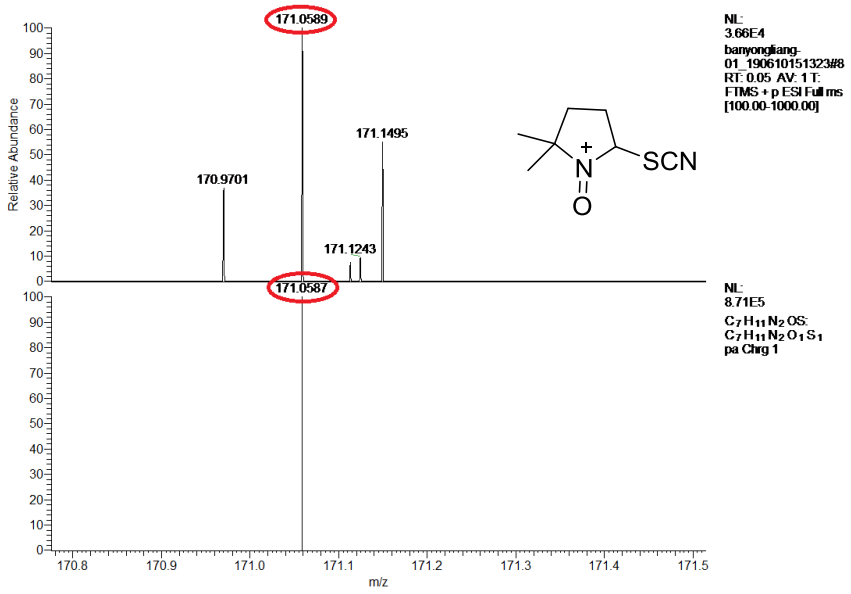


Figure S8. The HRMS spectrum of radical trapping experiments.

V. General Experimental Procedure for the Reaction

General Procedure for the Synthesis of Nitriles

To a 10 mL pyrex glass tube which equipped with a magnetic stirring bar were added aldoximes (1.0 equiv, 0.2 mmol), aizenuranine (2 mol %) and NH_4SCN (1.5 equiv, 0.3 mmol) in dry CH_3CN (2 mL). The reaction mixture was stirred at room temperature in the air and irradiated by 6 W blue LEDs. The reaction was monitored by TLC until aldoximes was no longer consumed (10 h). The solvent was removed under reduced pressure by rotary evaporator. Then, the residue was purified by silica gel column chromatography to give the desired product.

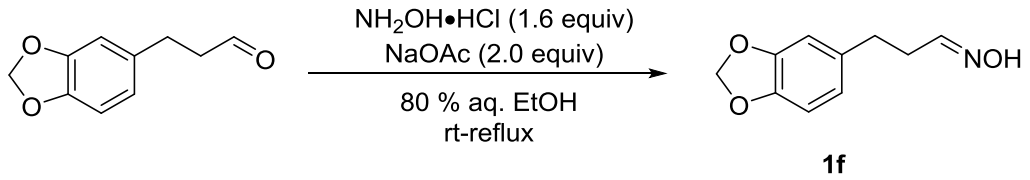
General Procedure for the Synthesis of Substrates

General Procedure for the Synthesis of Oximes [3]

A suspension of hydroxylamine hydrochloride (1.6 equiv), and NaOAc (2.0 equiv) in 80% aqueous EtOH (20 mL) was stirred at room temperature for 30 min. To this

solution, corresponding aldehyde (1.0 equiv) was added and the reaction mixture was heated gently to reflux for 1 h. After the completion of reaction by TLC, the reaction mass was cooled to rt followed by removal of excess ethanol under vacuum. The obtained residue was purified by column chromatography to obtain aldoximes.

Preparation of *(E/Z)*-3-(benzo[d][1,3]dioxol-5-yl)propanal oxime(1f)[3]

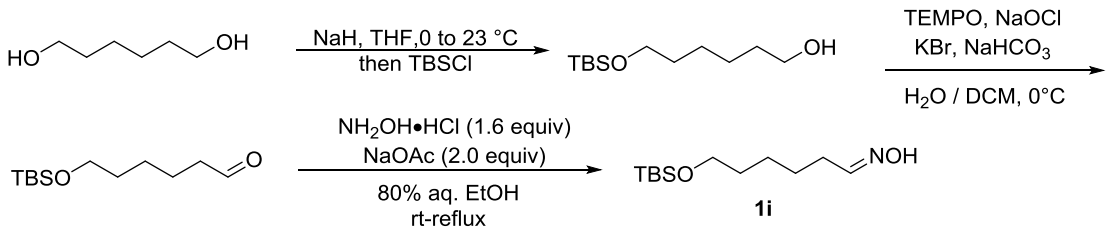


1f

A suspension of hydroxylamine hydrochloride (1.6 equiv), and NaOAc (2.0 equiv) in 80% aqueous EtOH (20 mL) was stirred at room temperature for 30 min. To this solution, corresponding aldehyde (1.0 equiv) was added and the reaction mixture was heated gently to reflux for 1 h. After the completion of reaction by TLC, the reaction mass was cooled to rt followed by removal of excess ethanol under vacuum. The obtained residue was purified by column chromatography to obtain corresponding aldoxime yielded the *E*/*Z*-mixture (60% *E*, 40% *Z*) white solid.

^{1}H NMR ($CDCl_3$, 400 MHz): δ ppm 7.47 (t, *J* = 5.4 Hz, 0.42H), 7.13 (t, *J* = 2.2 Hz, 2H), 7.07 (d, *J* = 3.2 Hz, 0.58H), 6.88 (q, *J* = 4.0 Hz, 2H), 4.91 (d, *J* = 3.2 Hz,1H), 4.66 (d, *J* = 5.2 Hz, 1H), 2.32 (s, 3H); **^{13}C NMR** ($CDCl_3$, 100 MHz): δ ppm 151.7, 151.3, 147.7, 145.9, 121.2, 108.8, 108.3, 100.9, 32.6, 31.7, 31.5, 26.7; **HRMS (ESI)** for Chemical Formula: $C_{10}H_{12}NO_3$ $(M+H)^+$ Calcd: 194.0812, Found: 194.0818.

Preparation of *(E/Z)*- 6-((tert-butyldimethylsilyl)oxy)hexanal oxime(1i)[3,4]



1i

6-((tert-butyldimethylsilyl)oxy)hexan-1-ol

To a solution of 1, 6-hexanediol (1.0 equiv) in THF (30 mL, 0.25 M) at 0 ℃ was added NaH (1.0 equiv). The reaction mixture was stirred at 0 ℃ for 30 min, then warmed to 23 ℃ and stirred for 3 h. TBSCl (1.0 equiv) was then added and the solution was stirred at 23 ℃ 16 h. The reaction mixture was poured into water (30 mL) and extracted with Et_2O (2 x 30 mL). The combined organic phases were dried over $MgSO_4$, and the solvent was removed by rotary evaporation, producing alcohol.

6-((tert-butyldimethylsilyl)oxy)hexanal

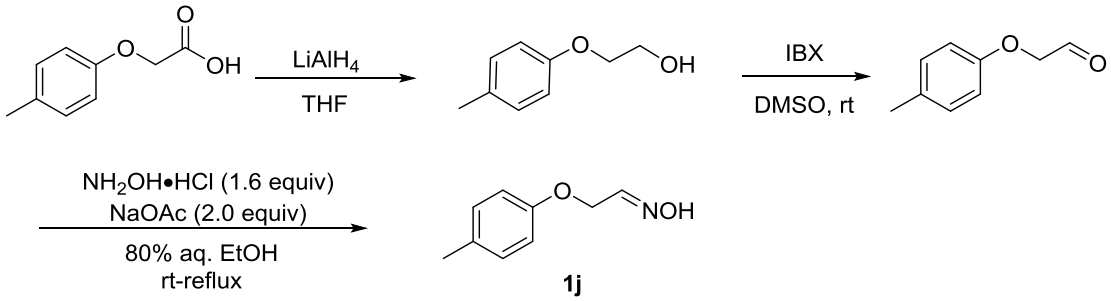
To a solution of alcohol (1.0 equiv) in DCM (25.0 mL, 0.4 M) at 0 ℃ was added TEMPO (0.01 equiv) A solution of KBr (0.011 equiv) in 5 % aq. $NaHCO_3$ (60 mL, 0.2 M) was then added to the organic phase, and the mixture was stirred vigorously at 0 ℃. NaOCl (1.1 equiv) was added dropwise, and the reaction mixture was stirred for 15 min. Upon completion, a saturated solution of $Na_2S_2O_3$ (15 mL) was added, and the mixture was stirred for 5 min. The mixture was extracted with DCM (2 x 25 mL), and the combined organic phases were washed with H_2O (50 mL) and brine (50 mL). The organic phase was dried over $MgSO_4$. The solvent was removed by rotary evaporation, producing aldehyde.

***(E/Z)*- 6-((tert-butyldimethylsilyl)oxy)hexanal oxime**

A suspension of hydroxylamine hydrochloride (1.6 equiv), and NaOAc (2.0 equiv) in 80 % aqueous EtOH (20 mL) was stirred at room temperature for 30 min. To this solution, corresponding aldehyde (1.0 equiv) was added and the reaction mixture was heated gently to reflux for 1 h. After the completion of reaction by TLC, the reaction mass was cooled to rt followed by removal of excess ethanol under vacuum. The obtained residue was purified by column chromatography to obtain corresponding aldoxime yielded the *E*/*Z*-mixture (58% *E*, 42% *Z*) colorless liquid.

^{1}H NMR ($CDCl_3$, 400 MHz): δ ppm 7.44 (t, *J* = 6.0 Hz, 0.54H), 6.73 (t, *J* = 5.4 Hz, 0.43H), 3.63 (m, 2H), 2.42 (m, 1H), 2.24 (m, 1H), 1.57 (m, 4H), 1.48 (m, 2H), 1.41 (s, 9H), 0.05 (s, 6H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ ppm 152.8, 152.2, 63.0, 32.5, 29.5, 26.35, 26.0, 25.9, 25.6, 25.4, 24.9, 18.3, -5.3; **HRMS (ESI)** for Chemical Formula: $C_{12}H_{28}NO_2Si$ $(M+H)^+$ Calcd: 246.1884, Found: 246.1892.

Preparation of *(E/Z)*-2-(p-tolyloxy) acetaldehyde oxime(1j)[3, 5, 6]



2-(p-tolyloxy) ethan-1-ol

To a cold (0 ℃) suspension of $LiAlH_4$ (2.5 equiv) in dry THF (40 mL) was added a solution of 2-(p-tolyloxy)acetic acid (1.0 equiv) in dry THF via an addition funnel. After the addition was complete, the cold bath was removed and the reaction mixture was stirred at r.t for 14 h, cooled to 0 ℃, carefully quenched with 1 N NaOH solution (1.25 mL) followed by H_2O (3.75 mL), and stirred at 0 ℃ for 1 h during which time a white precipitate formed. The precipitate was filtered off and washed with Et_2O (100 mL). The filtrate was concentrated under vacuum to leave a light yellow residue that was purified by column chromatography on silica gel to give the primary alcohol as colorless oil;

2-(p-tolyloxy) acetaldehyde

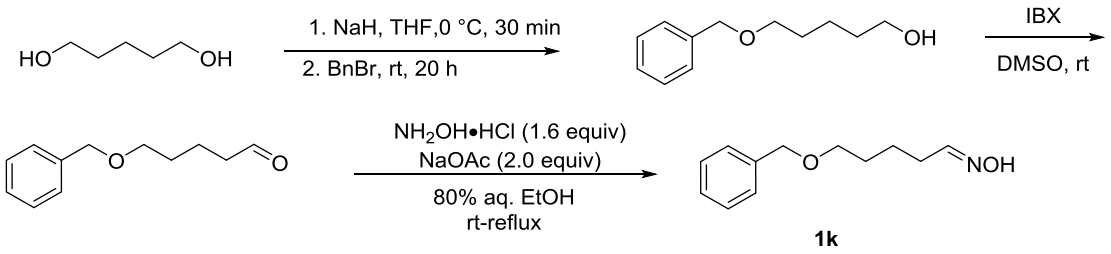
IBX (1.1 equiv) was stirred in DMSO (5 mL) vigorously until a clear solution was obtained. Then compound 2-(p-tolyloxy) ethan-1-ol (1.0 equiv) was added. After stirring for 4 h, the reaction mixture was purified by a flash column chromatography to afford 2-(p-tolyloxy) acetaldehyde.

***(E/Z)*-2-(p-tolyloxy) acetaldehyde oxime**

A suspension of hydroxylamine hydrochloride (1.6 equiv), and NaOAc (2.0 equiv) in 80% aqueous EtOH (20 mL) was stirred at room temperature for 30 min. To this solution, corresponding aldehyde (1.0 equiv) was added and the reaction mixture was heated gently to reflux for 1 h. After the completion of reaction by TLC, the reaction mass was cooled to rt followed by removal of excess ethanol under vacuum. The obtained residue was purified by column chromatography to obtain corresponding aldoxime yielded the *E*/*Z*-mixture (42% *E*, 58% *Z*) white solid.

^{1}H NMR ($CDCl_3$ 400 MHz): δ ppm 8.48 (brs, 1H), 7.66 (t, *J* = 5.4 Hz, 0.43H), 7.13(m, 2H), 7.06 (s, 0.56H),6.86 (t, *J* = 7.8 Hz, 2H), 4.90 (d, *J* = 3.2 Hz, 1H), 4.65 (d, *J* = 5.6 Hz, 1H), 2.31 (s, 3H); **^{13}C NMR:** ($CDCl_3$, 100 MHz) δ ppm 155.7, 150.3, 147.7, 130.7, 130.1, 114.6, 114.3, 65.9, 62.0, 20.4; **HRMS (ESI)** for Chemical Formula: $C_9H_{12}NO_2$ $(M+H)^+$ Calcd: 166.0863, Found: 166.0868.

Preparation of *(E/Z)*-5-(benzyloxy)pentanal oxime(1k)[3, 6, 7]



1k

5-(benzyloxy)pentan-1-ol

A solution of 1, 5-pentanediol (7.0 equiv) in THF (25 mL) was slowly added to a slurry of NaH (60% suspension in mineral oil, 1.2 equiv) in THF (12.5 mL) at 0 ℃ under nitrogen. After stirring for 30 min at 0 ℃ a solution of benzyl bromide (1.0 equiv) in THF (12.5 mL) was slowly added over 10 min. The reaction was warmed to room temperature and stirred for 20 h. Water was added (5 mL) and THF was removed under reduced pressure to oil that was divided between water (100 mL) and EtOAc (25 mL). The layers were separated and the aqueous phase was extracted with EtOAc (3 x 25 mL). The combined organic layers were washed with water (5 x 10 mL) and finally with brine, dried over sodium sulfate and concentrated to afford colorless liquid.

5-(benzyloxy)pentanal

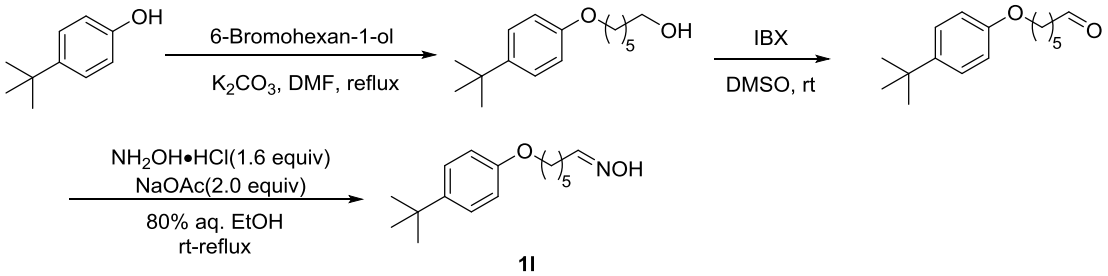
IBX (1.1 equiv) was stirred in DMSO (5 mL) vigorously until a clear solution was obtained. Then compound 6-Bromohexan-1-ol (1.0 equiv) was added. After stirring for 4 h, the reaction mixture was purified by a flash column chromatography to afford 5-(benzyloxy)pentanal.

***(E/Z)*-5-(benzyloxy)pentanal oxime**

A suspension of hydroxylamine hydrochloride (1.6 equiv), and NaOAc (2.0 equiv) in 80% aqueous EtOH (20 mL) was stirred at room temperature for 30 min. To this solution, corresponding aldehyde (1.0 equiv) was added and the reaction mixture was heated gently to reflux for 1 h. After the completion of reaction by TLC, the reaction mass was cooled to rt followed by removal of excess ethanol under vacuum. The obtained residue was purified by column chromatography to obtain corresponding aldoxime yielded the *E*/*Z*-mixture (55% *E*, 45% *Z*) colorless liquid.

^{1}H NMR ($CDCl_3$, 400 MHz): δ ppm 8.39 (brs, 1H), 7.43 (q, *J* = 6.0 Hz, 0.54H), 7.34 (m, 5H), 6.73 (t, *J* = 5.4 Hz, 0.45H), 4.50 (d, *J* = 2.4 Hz, 2H), 3.50 (dd, *J* = 5.8 Hz, 2H), 2.43 (m, 1H), 2.24 (m, 1H), 1.69 (m, 4H); **^{13}C NMR** ($CDCl_3$, 100 MHz): δ ppm 152.4, 151.8, 138.4, 128.3, 127.6, 127.5, 72.9, 69.7, 29.4, 29.2, 29.1, 24.7, 23.2, 22.7. **MS (ESI, m/z):** Calculated for $[C_{12}H_{17}NO_2]$ $(M+H)^+$ 208.1 found 208.3.

Preparation of *(E/Z)*-6-(4-(tert-butyl)phenoxy)hexanal oxime(1l) [3, 6, 8]



1l

6-(4-(tert-butyl)phenoxy)hexan-1-ol

A mixture of 1-Hydroxy-4-tert-butylbenzene (1.0 equiv), 6-bromohexan-1-ol (1.0 equiv), and potassium carbonate (2.0 equiv) in dry dimethylformamide (50 mL) was heated under reflux for 4 h. The reaction mixture was allowed to cool to room temperature. Water (80 mL) was added and the aqueous phase was extracted with ether (3×50 mL). The combined organic layers were washed twice with water after with 2 M NaOH and finally dried over $MgSO_4$. The product was collected by filtration as a white solid and used in the next step without further purification.

6-(4-(tert-butyl)phenoxy)hexanal

IBX (1.1 equiv) was stirred in DMSO (5 mL) vigorously until a clear solution was obtained. Then compound 6-Bromohexan-1-ol (1.0 equiv) was added. After stirring

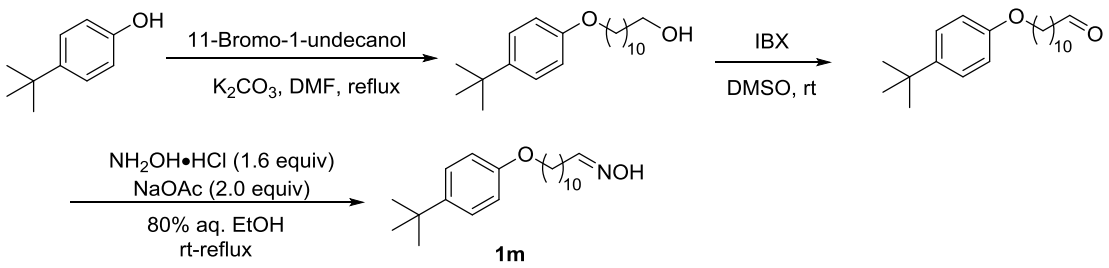
for 4 h, the reaction mixture was purified by a flash column chromatography to afford 6-(4-(tert-butyl)phenoxy)hexanal.

***(E/Z)*-6-(4-(tert-butyl)phenoxy)hexanal oxime**

A suspension of hydroxylamine hydrochloride (1.6 equiv) and NaOAc (2.0 equiv) in 80% aqueous EtOH (20 mL) was stirred at room temperature for 30 min. To this solution, corresponding aldehyde (1.0 equiv) was added and the reaction mixture was heated gently to reflux for 1 h. After the completion of reaction by TLC, the reaction mass was cooled to rt followed by removal of excess ethanol under vacuum. The obtained residue was purified by column chromatography to obtain corresponding aldoxime yielded the *E*/*Z*-mixture (57% *E*, 43% *Z*) white solid.

^{1}H NMR ($CDCl_3$, 400 MHz): δ ppm 8.59 (brs, 0.66H), 7.47 (q, *J* = 1.9 Hz, 0.57H), 7.33 (d, *J* = 8.0 Hz, 2H), 6.87 (d, *J* = 6.0 Hz, 2H), 6.78 (t, *J* = 5.0 Hz, 0.43H), 3.96 (s, 2H), 2.45 (d, *J* = 5.6 Hz, 1H), 2.26 (s, 1H), 1.81 (s, 2H), 1.60 (t, *J* = 5.0 Hz, 4H), 1.32 (t, *J* = 2.4 Hz, 9H); **^{13}C NMR** ($CDCl_3$, 100 MHz): δ ppm 156.7, 152.0, 143.2, 126.1, 113.9, 67.5, 34.0, 31.5, 29.4, 29.0, 26.3, 25.9, 25.8, 25.6, 24.9; **HRMS (ESI)** for Chemical Formula: $C_{16}H_{26}NO_2$ $(M+H)^+$ Calcd: 264.1958, Found: 264.1963.

Preparation of *(E/Z)*-11-(4-(tert-butyl)phenoxy)undecanal oxime(1m) [3, 6, 8]



11-(4-(tert-butyl)phenoxy)undecan-1-ol

A mixture of 1-Hydroxy-4-tert-butylbenzene (1.0 equiv), 11-bromoundecanol (1.0 equiv), and potassium carbonate (2.0 equiv) in dry dimethylformamide (50 mL) was heated under reflux for 4 h. The reaction mixture was allowed to cool to room temperature. Water (80 mL) was added and the aqueous phase was extracted with ether (3×50 mL). The combined organic layers were washed twice with water after

with 2 M NaOH and finally dried over $MgSO_4$. The product was collected by filtration as a white solid and used in the next step without further purification.

11-(4-(tert-butyl)phenoxy)undecanal

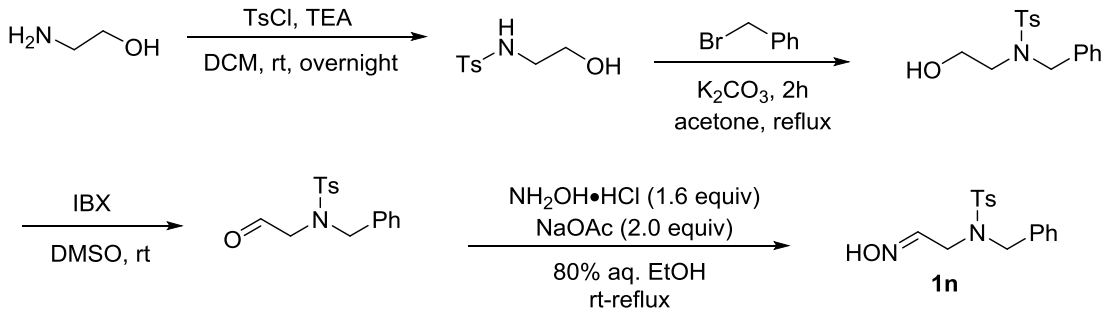
IBX (1.1 equiv) was stirred in DMSO (5 mL) vigorously until a clear solution was obtained. Then compound 11-(4-(tert-butyl)phenoxy)undecan-1-ol (1.0 equiv) was added. After stirring for 4 h, the reaction mixture was purified by a flash column chromatography to afford 11-(4-(tert-butyl)phenoxy)undecanal.

***(E/Z)*-11-(4-(tert-butyl)phenoxy)undecanal oxime**

A suspension of hydroxylamine hydrochloride (1.6 equiv), and NaOAc (2.0 equiv) in 80% aqueous EtOH (20 mL) was stirred at room temperature for 30 min. To this solution, corresponding aldehyde (1.0 equiv) was added and the reaction mixture was heated gently to reflux for 1 h. After the completion of reaction by TLC, the reaction mass was cooled to rt followed by removal of excess ethanol under vacuum. The obtained residue was purified by column chromatography to obtain corresponding aldoxime yielded the *E*/*Z*-mixture (50% *E*, 50% *Z*) white solid.

^{1}H NMR ($CDCl_3$, 400 MHz): δ ppm 7.46 (t, *J* = 6.2 Hz, 0.51H), 7.32 (t, *J* = 9.4 Hz, 2H), 6.86 (d, *J* = 8.8 Hz, 2H), 6.75 (t, *J* = 5.4 Hz, 0.51H), 3.96 (t, *J* = 6.6 Hz, 2H), 2.42 (m, 2H), 1.81(m, 2H), 1.52 (d, *J* = 6.8 Hz, 4H), 1.49 (m, 19H); **^{13}C NMR** ($CDCl_3$, 100 MHz): δ ppm 156.9, 153.1, 152.4, 143.1, 126.1, 113.9, 67.9, 34.0, 31.5, 29.5, 29.4, 29.3, 29.1, 26.5, 26.1, 24.9; **HRMS (ESI)** for Chemical Formula: $C_{21}H_{36}NO_2$ $(M+H)^+$ Calcd: 334.2741, Found: 334.2747.

Preparation of *(E/Z)*-N-benzyl-N-(2-(hydroxyimino)ethyl)-4-methylbenzenesulfonamide(1n)[3, 6, 9]



N-(2-hydroxyethyl)-4-methylbenzenesulfonamide

To a solution of 2-Aminoethanol (12.2 g, 200 mmol, 1.0 equiv) in DCM (150 mL) at room temperature was added TsCl (38.0 g, 200 mmol, 1.0 equiv). Then a solution of triethylamine (22.2 g, 220 mmol, 1.1 equiv) in 50 mL DCM was added dropwise by constant pressure funnel under vigorous stirring. The mixture was stirred at room temperature overnight and then washed with water (50 mL × 3). The organic layer was dried over Na_2SO_4 and concentrated to afford the crude alcohol as a white solid, which was used without further purification.

N-benzyl-N-(2-hydroxyethyl)-4-methylbenzenesulfonamide

A mixture of N-(2-hydroxyethyl)-4-methyl-N-(prop-2-yn-1-yl) benzenesulfon amide (1.0 equiv), (bromomethyl) benzene (1.0 equiv) and K_2CO_3 (1.5 equiv) in acetone (10 mL) was refluxed for 2 h (the reaction was monitored by TLC). After cooling to room temperature, the reaction mixture was filtered, concentrated and purified by a flash column chromatography to afford the product.

N-benzyl-4-methyl-N-(2-oxoethyl)benzenesulfonamide

IBX (1.1 equiv) was stirred in DMSO (5 mL) vigorously until a clear solution was obtained. Then compound N-benzyl-N-(2-hydroxyethyl)-4-methylbenzenesulfon-amide (1.0 equiv) was added. After stirring for 4 h, the reaction mixture was purified by a flash column chromatography to afford N-benzyl-4-methyl-N-(2-oxoethyl) benzenesulfonamide.

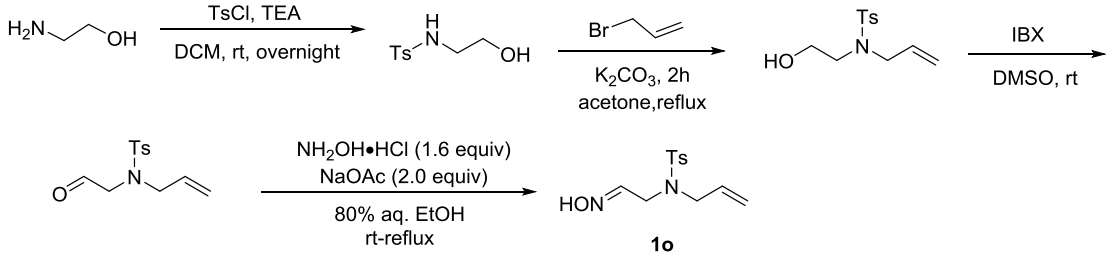
***(E/Z)*-N-benzyl-N-(2-(hydroxyimino) ethyl)-4-methylbenzenesulfonamide**

A suspension of hydroxylamine hydrochloride (1.6 equiv), and NaOAc (2.0 equiv) in 80% aqueous EtOH (20 mL) was stirred at room temperature for 30 min. To this solution, corresponding aldehyde (1.0 equiv) was added and the reaction mixture was heated gently to reflux for 1 h. After the completion of reaction by TLC, the reaction mass was cooled to rt followed by removal of excess ethanol under vacuum. The obtained residue was purified by column chromatography to obtain corresponding aldoxime yielded the *E*/*Z*-mixture (61% *E*, 39% *Z*) white solid.

^{1}H NMR ($CDCl_3$, 400 MHz): δ ppm 7.76 (dd, *J* = 4.0 Hz, 2H), 7.36 (m, 7.5H), 7.09 (t,

J = 4.0 Hz, 0.56H), 6.51 (t, *J* = 4.1 Hz, 0.45H), 4.32 (d, *J* = 4.4 Hz, 2H), 4.01 (d, *J* = 4.0 Hz, 1H), 3.83 (d, *J* = 6.0 Hz, 1H), 2.45 (s, 3H); **^{13}C NMR** ($CDCl_3$, 100 MHz): δ ppm 146.9, 143.8, 135.3, 135.2, 123.0, 129.9, 128.8, 128.7, 128.6, 128.2, 128.0, 127.3, 53.1, 51.4, 45.6, 42.7, 21.5; **HRMS (ESI)** for Chemical Formula: $C_{16}H_{19}N_2O_3S$ $(M+H)^+$ Calcd: 319.1111, Found: 319.1118.

Preparation of *(E/Z)*-N-allyl-N-(2-(hydroxyimino)ethyl)-4-methylbenzenesulfonamide(1o)[3, 6, 9]



N-(2-hydroxyethyl)-4-methylbenzenesulfonamide

To a solution of 2-Aminoethanol (12.2 g, 200 mmol, 1.0 equiv) in DCM (150 mL) at room temperature was added TsCl (38.0 g, 200 mmol, 1.0 equiv). Then a solution of triethylamine (22.2 g, 220 mmol, 1.1 equiv) in 50 mL DCM was added dropwise by constant pressure funnel under vigorous stirring. The mixture was stirred at room temperature overnight and then washed with water (50 mL × 3). The organic layer was dried over Na_2SO_4 and concentrated to afford the crude alcohol as a white solid, which was used without further purification.

N-allyl-N-(2-hydroxyethyl)-4-methylbenzenesulfonamide

A mixture of N-(2-hydroxyethyl)-4-methylbenzenesulfonamide (1.0 equiv), allyl bromide (1.0 equiv) and K_2CO_3 (1.5 equiv) in acetone was refluxed for 2 h (the reaction was monitored by TLC). After cooling to room temperature, the reaction mixture was filtered, concentrated and purified by a flash column chromatography to afford the product.

N-allyl-4-methyl-N-(2-oxoethyl)benzenesulfonamide

IBX (1.1 equiv) was stirred in DMSO (5 mL) vigorously until a clear solution was obtained. Then compound N-allyl-N-(2-hydroxyethyl)-4-methylbenzenesulfon amide

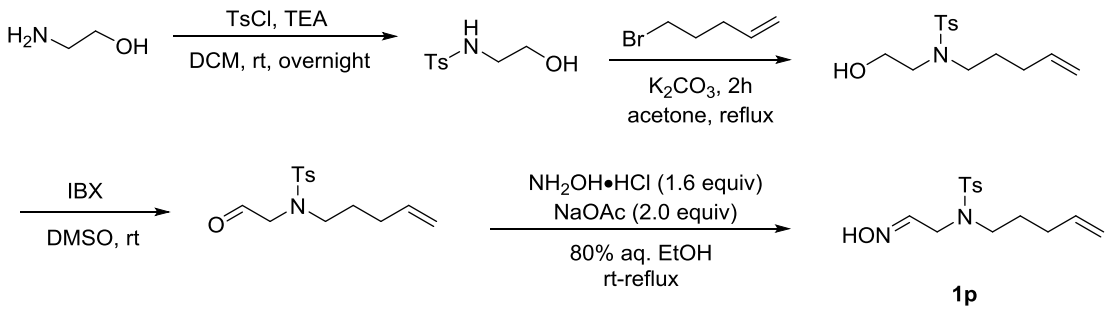
(1.0 equiv) was added. After stirring for 4 h, the reaction mixture was purified by a flash column chromatography to afford N-allyl-4-methyl-N-(2-oxoethyl) benzenesulfonamide as a Light yellow liquid.

***(E/Z)*-N-allyl-N-(2-(hydroxyimino)ethyl)-4-methylbenzenesulfonamide**

A suspension of hydroxylamine hydrochloride (1.6 equiv), and NaOAc (2.0 equiv) in 80% aqueous EtOH (20 mL) was stirred at room temperature for 30 min. To this solution, corresponding aldehyde (1.0 equiv) was added and the reaction mixture was heated gently to reflux for 1 h. After the completion of reaction by TLC, the reaction mass was cooled to rt followed by removal of excess ethanol under vacuum. The obtained residue was purified by column chromatography to obtain corresponding aldoxime yielded the *E*/*Z*-mixture (58% *E*, 42% *Z*) white solid.

^{1}H NMR ($CDCl_3$, 400 MHz): δ ppm 8.45 (s,1H), 7.72 (d, *J* = 8.0 Hz, 2H), 7.34 (dd, *J* = 7.9 Hz, 2H), 7.26 (t, *J* = 5.8 Hz , 0.62H) , 6.76 (t, *J* = 4.2 Hz , 0.46H) ,5.73 (m, 1H), 5.22 (m, 2H), 4.06 (d, *J* = 4.0 Hz, 1H), 3.90 (d, *J* = 2.0 Hz , 1H), 3.80 (d, *J* = 6.4 Hz, 2H), 2.44 (s, 3H); **^{13}C NMR** ($CDCl_3$, 100 MHz): δ ppm 149.4, 147.2, 143.8, 143.7, 136.5, 135.9, 129.9, 127.2, 120.0, 119.8, 52.1, 50.3, 45.5, 42.4, 21.5; **HRMS (ESI)** for Chemical Formula: $C_{12}H_{17}N_2O_3S$ $(M+H)^+$ Calcd: 269.0954, Found: 269.0961.

Preparation of *(E/Z)*-N-(2-(hydroxyimino)ethyl)-4-methyl-N-(pent-4-en-1-yl) benzenesulfonamide(1p)[3, 6, 9]



N-(2-hydroxyethyl)-4-methylbenzenesulfonamide

To a solution of 2-Aminoethanol (12.2 g, 200 mmol, 1.0 equiv) in DCM (150 mL) at room temperature was added TsCl (38.0 g, 200 mmol, 1.0 equiv). Then a solution

of triethylamine (22.2 g, 220 mmol, 1.1 equiv) in 50 mL DCM was added dropwise by constant pressure funnel under vigorous stirring. The mixture was stirred at room temperature overnight and then washed with water (50 mL × 3). The organic layer was dried over Na_2SO_4 and concentrated to afford the crude alcohol as a white solid, which was used without further purification.

N-(2-hydroxyethyl)-4-methyl-N-(pent-4-en-1-yl)benzenesulfonamide

A mixture of N-(2-hydroxyethyl)-4-methyl-N-(prop-2-yn-1-yl) benzenesul fonamide (1.0 equiv), 5-bromopent-1-ene (1.0 equiv) and K_2CO_3 (1.5 equiv) in acetone (10 mL) was refluxed for 2 h (the reaction was monitored by TLC). After cooling to room temperature, the reaction mixture was filtered, concentrated and purified by a flash column chromatography to afford the product.

4-Methyl-N-(2-oxoethyl)-N-(pent-4-en-1-yl)benzenesulfonamide

IBX (1.1 equiv) was stirred in DMSO (5 mL) vigorously until a clear solution was obtained. Then compound N-(2-hydroxyethyl)-4-methyl-N-(3-methylbut- 2-en-1-yl) benzenesulfonamide (1.0 equiv) was added. After stirring for 4 h, the reaction mixture was purified by a flash column chromatography to afford 4-methyl-N-(3-methylbut-2-en-1-yl)-N-(2-oxoethyl) benzenesulfon- amide.

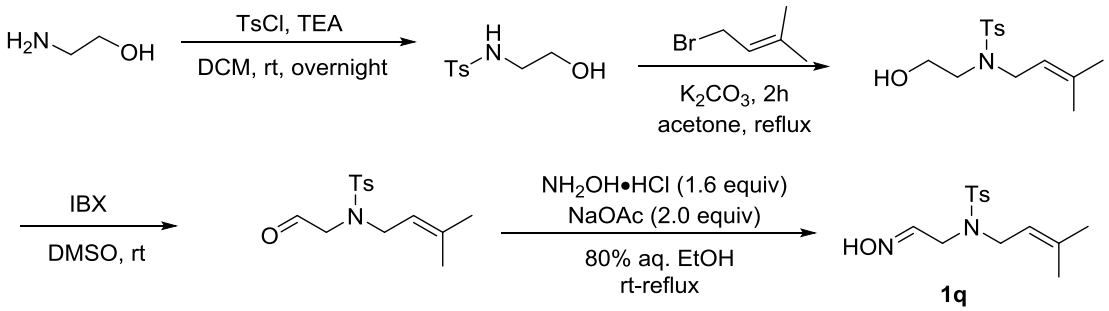
***(E/Z-)*N-(2-(hydroxyimino)ethyl)-4-methyl-N-(pent-4-en-1-yl)benzenesulfonamide**

A suspension of hydroxylamine hydrochloride (1.6 equiv), and NaOAc (2.0 equiv) in 80% aqueous EtOH (20 mL) was stirred at room temperature for 30 min. To this solution, corresponding aldehyde (1.0 equiv) was added and the reaction mixture was heated gently to reflux for 1 h. After the completion of reaction by TLC, the reaction mass was cooled to rt followed by removal of excess ethanol under vacuum. The obtained residue was purified by column chromatography to obtain corresponding aldoxime yielded the *E*/*Z*-mixture (61% *E*, 39% *Z*) white solid.

^{1}H NMR ($CDCl_3$, 400 MHz): δ ppm 7.70 (d, *J* = 8.0 Hz, 2H), 7.33 (t, *J* = 4.0 Hz, 2H), 7.27 (t, *J* = 3.0 Hz, 0.68H), 6.75 (t, *J* = 5.6 Hz, 0.43H), 5.81 (m, 1H), 5.04 (m, 2H), 4.08 (d, *J* = 4.4 Hz, 1H), 3.90 (d, *J* = 2.0 Hz, 1H), 3.17 (dd, *J* = 15.0 Hz, 2H), 2.43 (s,

3H), 2.11 (m, 2H), 1.68 (m, 2H); **^{13}C NMR** ($CDCl_3$, 100 MHz): δ ppm 149.5, 147.5, 143.7, 137.2, 136.4, 135.9, 129.9, 127.1, 115.5, 49.0, 47.6, 46.6, 43.1, 30.5, 27.2, 21.5; **HRMS (ESI)** for Chemical Formula: $C_{14}H_{21}N_2O_3S$ $(M+H)^+$ Calcd: 297.1267, Found: 297.1274.

Preparation of (*E/Z*) -N-(2-(hydroxyimino) ethyl)-4-methyl-N-(3-methylbut-2-en -1-yl) benzenesulfonamide(1q)[3, 6, 9]



N-(2-hydroxyethyl)-4-methylbenzenesulfonamide

To a solution of 2-Aminoethanol (12.2 g, 200 mmol, 1.0 equiv) in DCM (150 mL) at room temperature was added TsCl (38.0 g, 200 mmol, 1.0 equiv). Then a solution of triethylamine (22.2 g, 220 mmol, 1.1 equiv) in 50 mL DCM was added dropwise by constant pressure funnel under vigorous stirring. The mixture was stirred at room temperature overnight and then washed with water (50 mL × 3). The organic layer was dried over Na_2SO_4 and concentrated to afford the crude alcohol as a white solid, which was used without further purification.

N-(2-hydroxyethyl)-4-methyl-N-(3-methylbut-2-en-1-yl) benzenesulfonamide

A mixture of N-(2-hydroxyethyl)-4-methyl-N-(prop-2-yn-1-yl)benzenesul fonamide (1.0 equiv), 1-bromo-3-methylbut-2-ene (1.0 equiv) and K_2CO_3 (1.5 equiv) in acetone (10 mL) was refluxed for 2 h (the reaction was monitored by TLC). After cooling to room temperature, the reaction mixture was filtered, concentrated and purified by a flash column chromatography to afford the product.

4-methyl-N-(3-methylbut-2-en-1-yl)-N-(2-oxoethyl) benzenesulfonamide

IBX (1.1 equiv) was stirred in DMSO (5 mL) vigorously until a clear solution was obtained. Then compound N-(2-hydroxyethyl)-4-methyl-N-(3-methylbut-2-en-1-yl)

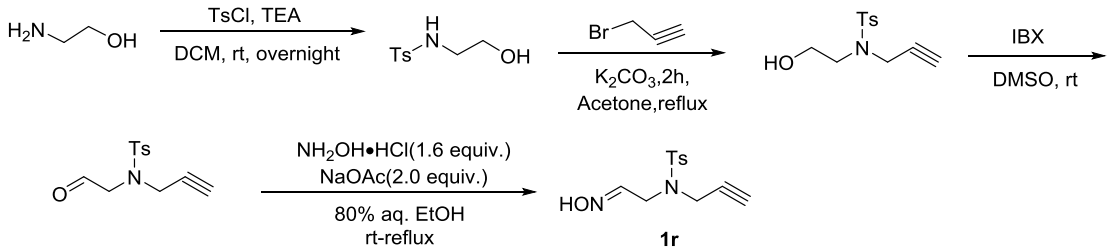
benzenesulfonamide (1.0 equiv) was added. After stirring for 4 h, the reaction mixture was purified by a flash column chromatography to afford 4-methyl-N-(3-methylbut-2-en-1-yl)-N-(2-oxoethyl) benzenesulfonamide.

***(E/Z)*-N-(2-(hydroxyimino)ethyl)-4-methyl-N-(3-methylbut-2-en-1-yl)benzenesulfonamide**

A suspension of hydroxylamine hydrochloride (1.6 equiv), and NaOAc (2.0 equiv) in 80% aqueous EtOH (20 mL) was stirred at room temperature for 30 min. To this solution, corresponding aldehyde (1.0 equiv) was added and the reaction mixture was heated gently to reflux for 1 h. After the completion of reaction by TLC, the reaction mass was cooled to rt followed by removal of excess ethanol under vacuum. The obtained residue was purified by column chromatography to obtain corresponding aldoxime yielded the *E*/*Z*-mixture (54% *E*, 46% *Z*) white solid.

^{1}H NMR ($CDCl_3$, 400 MHz): δ ppm 8.52 (brs, 1H), 7.40 (t, *J* = 4.0 Hz, 2H), 7.33 (m, 2H), 7.26 (s, 0.54H), 6.74 (s, 0.46H), 5.01 (m, 1H) ,4.02 (d, *J* = 4.0 Hz, 1H), 3.86 (d, *J* = 5.6 Hz, 1H), 3.79 (t, *J* = 6.0 Hz, 2H), 2.43 (s, 3H), 1.67 (s, 3H), 1.59 (s, 3H); **^{13}C NMR** ($CDCl_3$, 100 MHz): δ ppm 149.8, 143.6, 138.6, 138.0, 136.1, 129.8, 127.3, 117.9, 46.7, 45.6, 45.4, 42.4, 25.7, 21.5, 17.7; **HRMS (ESI)** for Chemical Formula: $C_{14}H_{21}N_2O_3S$ $(M+H)^+$ Calcd: 297.1267,Found: 297.1273.

Preparation of *E/Z*-N-(2-(hydroxyimino)ethyl)-4-methyl-N-(prop-2-yn-1-yl) benzenesulfon-amide(1r)[1, 4, 7]



N-(2-hydroxyethyl)-4-methylbenzenesulfonamide

To a solution of 2-Aminoethanol (12.2 g, 200 mmol, 1.0 equiv) in DCM (150 mL) at room temperature was added TsCl (38.0 g, 200 mmol, 1.0 equiv). Then a solution

of triethylamine (22.2 g, 220 mmol, 1.1 equiv) in 50 mL DCM was added dropwise by constant pressure funnel under vigorous stirring. The mixture was stirred at room temperature overnight and then washed with water (50 mL × 3). The organic layer was dried over Na_2SO_4 and concentrated to afford the crude alcohol as a white solid, which was used without further purification.

N-(2-hydroxyethyl)-4-methyl-N-(prop-2-yn-1-yl)benzenesulfonamide

A mixture of N-(2-hydroxyethyl)-4-methylbenzenesulfonamide (1.0 equiv), 3-bromoprop-1-yne (1.0 equiv) and K_2CO_3 (1.5 equiv) in acetone (10 mL) was refluxed for 2 h (the reaction was monitored by TLC). After cooling to room temperature, the reaction mixture was filtered, concentrated and purified by a flash column chromatography to afford the product.

4-Methyl-N-(2-oxoethyl)-N-(prop-2-yn-1-yl)benzenesulfonamide

IBX (1.1 equiv) was stirred in DMSO (5 mL) vigorously until a clear solution was obtained. Then compound N-(2-hydroxyethyl)-4-methyl-N-(prop-2-yn-1-yl)benzene-sulfonamide (1.0 equiv) was added. After stirring for 4 h, the reaction mixture was purified by a flash column chromatography to afford 4-Methyl-N- (2-oxoethyl)-N-(prop-2-yn-1-yl) benzenesulfonamide.

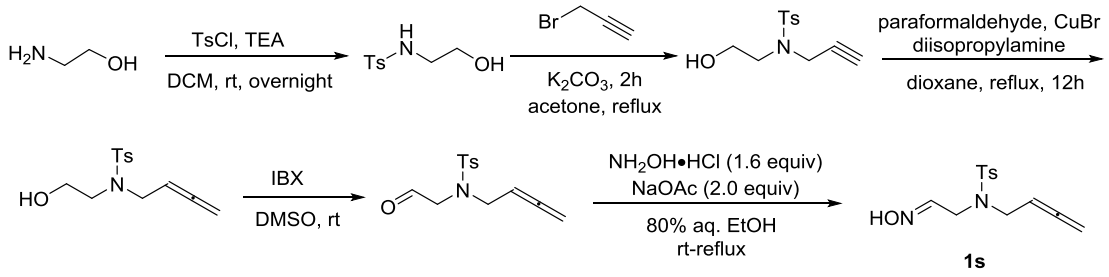
***(E/Z)*-N-(2-(hydroxyimino)ethyl)-4-methyl-N-(prop-2-yn-1-yl)benzenesulfonamide**

A suspension of hydroxylamine hydrochloride (1.6 equiv), and NaOAc (2.0 equiv) in 80% aqueous EtOH (20 mL) was stirred at room temperature for 30 min. To this solution, corresponding aldehyde (1.0 equiv) was added and the reaction mixture was heated gently to reflux for 1 h. After the completion of reaction by TLC, the reaction mass was cooled to rt followed by removal of excess ethanol under vacuum. The obtained residue was purified by column chromatography to obtain corresponding aldoxime yielded the *E*/*Z*-mixture (60% *E*, 40% *Z*) white solid.

^{1}H NMR ($CDCl_3$, 400 MHz): δ ppm 7.75 (t, *J* = 4.2 Hz, 2H), 7.40 (t, *J* = 5.8 Hz, 0.6H), 7.34 (dd, *J* = 4.1 Hz, 2H), 6.88 (t, *J* = 4.2 Hz, 0.4H), 4.18 (m, 3H), 3.98 (d, *J* = 6.0 Hz, 1H), 2.44 (s, 3H), 2.12 (m, 1H); **^{13}C NMR** ($CDCl_3$, 100 MHz): δ ppm 148.7,

146.5, 144.1, 144.0, 129.7, 127.7, 76.2, 74.4, 74.3, 45.4, 42.4, 38.4, 36.9, 21.6; **HRMS (ESI)** for Chemical Formula: $C_{12}H_{15}N_2O_3S$ $(M+H)^+$ Calcd: 289.0617, Found: 289.0621.

Preparation of *(E/Z)*-N-N-(buta-2, 3-dien-1-yl)-N-(2-(hydroxyimino)ethyl)-4-methylbenzene- sulfonamide(1s)[3, 6, 9,10]



N-(2-hydroxyethyl)-4-methylbenzenesulfonamide

To a solution of 2-Aminoethanol (12.2 g, 200 mmol, 1.0 equiv) in DCM (150 mL) at room temperature was added TsCl (38.0 g, 200 mmol, 1.0 equiv). Then a solution of triethylamine (22.2 g, 220 mmol, 1.1 equiv) in 50 mL DCM was added dropwise by constant pressure funnel under vigorous stirring. The mixture was stirred at room temperature overnight and then washed with water (50 mL × 3). The organic layer was dried over Na_2SO_4 and concentrated to afford the crude alcohol as a white solid, which was used without further purification.

N-(2-hydroxyethyl)-4-methyl-N-(prop-2-yn-1-yl)benzenesulfonamide

A mixture of N-(2-hydroxyethyl)-4-methylbenzenesulfonamide (1.0 equiv), 3-bromoprop-1-yne (1.0 equiv) and K_2CO_3 (1.5 equiv) in acetone (10 mL) was refluxed for 2 h (the reaction was monitored by TLC). After cooling to room temperature, the reaction mixture was filtered, concentrated and purified by a flash column chromatography to afford the product.

N-(buta-2,3-dien-1-yl)-N-(2-hydroxyethyl)-4-methylbenzenesulfonamide

A suspension of N-(2-hydroxyethyl)-4-methyl-N-(prop-2-yn-1-yl)benzenesulfonamide (1.0 equiv), cuprous bromide (0.5 equiv), paraformaldehyde (2.5 equiv) and diisopropylamine (2.0 equiv) in dioxane (50 mL) was gently heated at reflux and

stirred for 12 h, cooled to room temperature, and filtered through a Celite pad. The dark-brown filtrate was concentrated in vacuo to a gummy residue and then diluted with 30 mL of water followed by addition of 50 mL of ether and acidified with 6N hydrochloric acid to pH 2. The ether-water layers were decanted from any residues, the ether layer was separated, and the aqueous solution was extracted with ether (5x20 mL). The ether extracts were combined and washed with a small portion of water until was reached to pH 6.5. The organic layer was then washed with brine, dried over $MgSO_4$ and concentrated. The crude product was separated by silca gel column chromatography.

N-(buta-2,3-dien-1-yl)-4-methyl-N-(2-oxoethyl)benzenesulfonamide

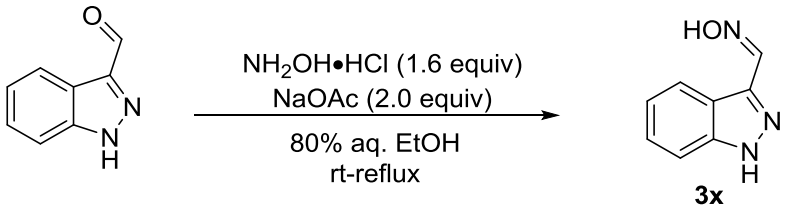
IBX (1.1 equiv) was stirred in DMSO (5 mL) vigorously until a clear solution was obtained. Then compound N-(buta-2, 3-dien-1-yl)-N-(2-hydroxyethyl)-4-methyl benzenesulfonamide (1.0 equiv) was added. After stirring for 4 h, the reaction mixture was purified by a flash column chromatography to afford N-(buta-2, 3-dien-1-yl)-4-methyl-N-(2-oxoethyl)benzenesulfonamide.

***(E/Z)*-N-N-(buta-2,3-dien-1-yl)-N-(2-(hydroxyimino)ethyl)-4-methylbenzenesulfonamide**

A suspension of hydroxylamine hydrochloride (1.6 equiv), and NaOAc (2.0 equiv) in 80% aqueous EtOH (20 mL) was stirred at room temperature for 30 min. To this solution, corresponding aldehyde (1.0 equiv) was added and the reaction mixture was heated gently to reflux for 1 h. After the completion of reaction by TLC, the reaction mass was cooled to rt followed by removal of excess ethanol under vacuum. The obtained residue was purified by column chromatography to obtain aldoxime yielded the *E*/*Z*-mixture (51% *E*, 49% *Z*) yellow solid.

^{1}H NMR ($CDCl_3$, 400 MHz): δ ppm 8.50 (brs, 1H), 7.72 (d, *J* = 7.2 Hz, 2H), 7.34 (t, *J* = 3.2 Hz, 2H), 7.31 (s, 0.46H), 6.80 (s, 0.49H), 5.00 (m, 1H), 4.75 (m, 2H), 3.95 (d, *J* = 6.0 Hz, 2H), 3.85 (dd, *J* = 4.0 Hz, 2H), 2.44 (s, 3H); **^{13}C NMR** ($CDCl_3$, 100 MHz): δ ppm 209.8, 209.7, 149.4, 147.3, 143.7, 129.8, 127.2, 85.4, 85.4, 48.4, 46.9, 45.7, 42.4, 21.5. **MS (ESI, m/z):** Calculated for $[C_{13}H_{16}N_2O_3S]$ $(M+H)^+$ 281.1 found 281.0.

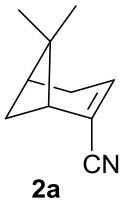
Preparation of (*E*)-1H-indazole-3-carbaldehyde oxime(3x)[3]



A suspension of hydroxylamine hydrochloride (1.6 equiv), and NaOAc (2.0 equiv) in 80% aqueous EtOH (20 mL) was stirred at room temperature for 30 min. To this solution, corresponding aldehyde (1.0 equiv) was added and the reaction mixture was heated gently to reflux for 1 h. After the completion of reaction by TLC, the reaction mass was cooled to rt followed by removal of excess ethanol under vacuum. The obtained residue was purified by column chromatography to obtain corresponding aldoxime yielded the *E* compound yellow solid.

^{1}H NMR (DMSO-d_6, 400 MHz): δ ppm 13.35 (s, 1H), 11.40 (s, 1H), 8.38 (s, 1H), 8.06 (d, J = 8.0 Hz, 1H), 7.58 (d, J = 8.4 Hz, 1H), 7.42 (t, J = 7.4 Hz, 1H), 7.22 (t, J = 7.6 Hz, 1H); **^{13}C NMR** (DMSO-d_6, 100 MHz): δ ppm 144.2, 141.2, 139.2, 126.8, 121.8, 121.5, 119.9, 110.5; **HRMS (ESI)** for Chemical Formula: $C_8H_7N_3O$ $(M+H)^+$ Calcd: 162.0662, Found: 162.0667.

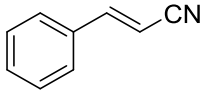
VI. Characterization Data of the Products



2a

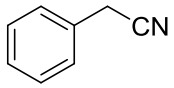
(1R,5S)-6,6-dimethylbicyclo[3.1.1]hept-2-ene-2-carbonitrile (2a)[11]**:** colorless liquid, 25.0 mg, (Yield: 85 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 6.55 (s, 1H), 2.54 (m, 4H), 2.16 (s, 1H), 1.32 (s, 3H); 1.25 (t, J = 4.6 Hz, 1H), 0.87 (s, 3H); **^{13}C NMR** (100 MHz,

$CDCl_3$): δ 142.1, 120.8, 118.4, 44.4, 39.7, 38.1, 32.5, 31.2, 25.6, 20.9; **MS (ESI, m/z):** Calculated for $[C_{10}H_{13}N]$ $(M+H)^+$ 148.1 found 148.1.



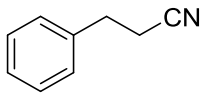
2b

cinnamonitrile (2b) [12]: yellow liquid, 17.0 mg, (Yield: 66 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.48 (m, 5H), 5.92 (d, *J* = 16.8 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 150.6, 133.5, 131.2, 129.1, 129.0, 127.3, 118.1, 96.3; **MS (ESI, m/z):** Calculated for $[C_9H_7N]$ $(M+H)^+$ 130.1 found 130.0.



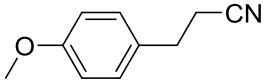
2c

2-phenylacetonitrilene (2c) [12]: yellow liquid, 14.7 mg, (Yield: 63 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.40 (m, 5H), 3.77 (s, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 129.9, 129.1, 128.0, 127.9, 117.8, 23.6; **MS (ESI, m/z):** Calculated for $[C_8H_7N]$ $(M+H)^+$ 118.1 found 118.0.



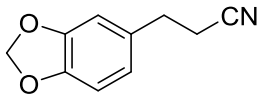
2d

3-phenylpropanenitrile (2d) [13]: colorless liquid, 23.2 mg, (Yield 74 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.33 (m, 5H), 2.96 (t, *J* = 7.4 Hz, 2H), 2.62 (t, *J* = 7.4 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 138.0, 128.8, 128.2, 127.2, 119.2, 31.5, 19.4; **MS (ESI, m/z):** Calculated for $[C_9H_9N]$ $(M+H)^+$ 132.1 found 132.1.



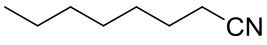
2e

3-(4-Methoxyphenyl)propanenitrile (**2e**)[13]: colorless liquid, 23.1 mg, (Yield 72 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.17 (d, *J* = 8.4 Hz, 2H), 6.89 (d, *J* = 8.8 Hz, 2H), 3.81 (s, 3H), 2.91 (t, *J* = 7.4 Hz, 2H), 2.59 (t, *J* = 7.4 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 158.7, 130.1, 129.3, 119.2, 114.2, 55.2, 30.7, 19.6; **MS (ESI, m/z):** Calculated for $[C_{10}H_{11}NO]$ $(M+H)^+$ 162.1 found 162.0.



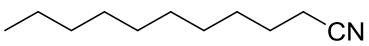
2f

3-(benzo[d][1,3]dioxol-5-yl)propanenitrile (2f)[14]: colorless liquid, 19.3 mg, (Yield: 55 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 6.79 (d, *J* = 7.6 Hz, 1H), 6.71 (m, 2H), 5.96 (s, 2H), 2.88 (t, *J* = 7.4 Hz, 2H), 2.59 (t, *J* = 7.4 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 147.9, 146.7, 131.7, 121.4, 119.1, 108.6, 101.1, 31.3, 19.7; **MS (ESI, m/z):** Calculated for $[C_{10}H_9NO_2]$ $(M+H)^+$ 175.1 found 175.1.



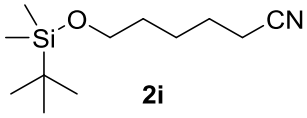
2g

octanenitrile (2g)[15]: colorless liquid, 24.2 mg, (Yield: 87 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 2.36 (t, *J* = 7.0 Hz, 2H), 1.66 (m, 2H), 1.46 (m, 2H), 1.41 (m, 6H), 1.28 (t, *J* = 3.4 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 119.9, 31.5, 28.6, 28.4, 25.3, 22.5, 17.1, 14.0; **MS (ESI, m/z):** Calculated for $[C_8H_{15}N]$ $(M+H)^+$ 126.1 found 126.1.



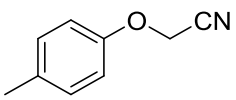
2h

undecanenitrile (2h)[16]: colorless liquid, 26.0 mg, (Yield: 78 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 2.33 (t, *J* = 7.2 Hz, 2H), 1.66 (m, 2H), 1.45 (q, *J* = 7.2 Hz, 2H), 1.29 (t, *J* = 6.8 Hz, 12H), 0.88 (t, *J* = 6.8 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 119.8, 31.8, 29.4, 29.3, 29.2, 28.7, 28.6, 25.3, 22.6, 17.1, 14.0; **MS (ESI, m/z):** Calculated for $[C_{11}H_{21}N]$ $(M+H)^+$ 168.2 found 168.1.



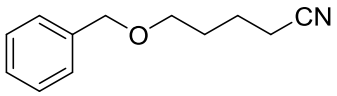
2i

6-((tert-butyldimethylsilyl)oxy)hexanenitrile (2i): colorless liquid, 33.1 mg, (Yield: 73 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 3.64 (t, *J* = 5.8 Hz, 2H), 2.37 (t, *J* = 7.2 Hz, 2H), 1.74 (dd, *J* = 7.2 Hz, 2H),1.66 (m, 4H), 0.90 (s, 9H), 0.06 (s, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 119.7, 63.6, 31.9, 25.9, 25.3, 25.2, 18.3, 17.1, -5.3; **HRMS (ESI)** for Chemical Formula: $C_{12}H_{26}NOSi$ $(M+H)^+$ Calcd: 228.1778; Found: 228.1785.



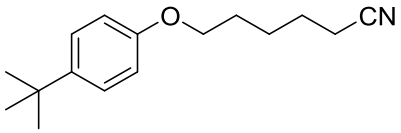
2j

2-(p-tolyloxy)acetonitrile (**2j**)[17]: yellow liquid, 21.2 mg, (Yield: 72 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.17 (d, *J* = 8.4 Hz, 2H), 6.91 (d, *J* = 8.4 Hz, 2H), 4.74 (s, 2H), 2.33 (s, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 154.5, 132.6, 130.3, 115.3, 115.0, 53.9, 20.6; **MS (ESI, m/z):** Calculated for $[C_9H_9NO]$ $(M+H)^+$ 148.1 found 147.9.



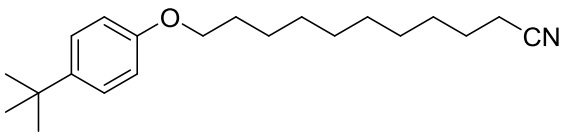
2k

5-(benzyloxy)pentanenitrile (2k): colorless liquid, 29.8 mg, (Yield: 79 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.39 (m, 5H), 4.51(s, *2*H), 3.54 (t, *J* = 5.6 Hz, 2H), 2.4 (t, *J* = 6.8 Hz, 2H), 1.82 (m, 4H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 138.2, 128.4, 127.6, 127.6, 119.7, 73.0, 68.9, 28.6, 22.5, 16.9; **HRMS (ESI)** for Chemical Formula: $C_{12}H_{16}NO$ $(M+H)^+$Calcd: 190.1226, Found: 190.1231.



2l

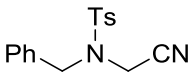
6-(4-(tert-butyl)phenoxy)hexanenitrile (2m): white solid, 37.3 mg (Yield: 76 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.33 (d, *J* = 8.8 Hz, 2H), 6.85 (d, *J* = 8.8 Hz, 2H), 3.99 (t, *J* = 6.2 Hz, 2H), 2.41 (t, *J* = 7.0 Hz, 2H), 1.87 (m, 2H), 1.78 (m, 2H), 1.69 (m, 2H) 1.32 (s, 9H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 156.6, 143.4, 126.2, 119.6, 113.9, 67.2, 34.0, 31.5, 28.5, 25.4, 25.2, 17.1; **HRMS (ESI)** for Chemical Formula: $C_{16}H_{24}NO$ $(M+H)^+$ Calcd: 246.1858, Found: 246.1858.



2m

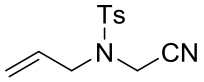
11-(4-(tert-butyl)phenoxy)undecanenitrile (2m): white solid, 50.4 mg (Yield: 80 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.30 (d, *J* = 8.8 Hz, 2H), 6.84 (d, *J* = 8.8 Hz, 2H),

3.95 (t, *J* = 6.6 Hz, 2H), 2.34 (t, *J* = 7.0 Hz, 2H), 1.80 (m, 2H), 1.68 (m, 2H), 1.46 (t, *J* = 6.4 Hz, 4H), 1.31 (d, *J* = 6.8 Hz, 17H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ156.8, 143.1, 126.1, 119.8, 113.9, 67.8, 34.0, 31.5, 29.4, 29.3, 29.3, 29.2, 28.7, 28.6, 26.0, 25.3, 17.1; **HRMS (ESI)** for Chemical Formula: $C_{21}H_{34}NO$ $(M+H)^+$ Calcd: 316.2635; Found: 316.2640.



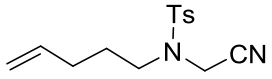
2n

N-benzyl-N-(cyanomethyl)-4-methylbenzenesulfonamide (2n): white solid, 46.2 mg (Yield: 77 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.83(d, *J* = 8.4 Hz, 2H), 7.43 (d, *J* = 8.0 Hz, 2H), 7.38 (m, 5H), 4.35 (s, 2H), 4.05 (s, 2H), 2.49 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 144.8, 134.2, 133.3, 130.1, 129.1, 128.8, 127.6, 113.1, 51.0, 34.2, 21.6; **HRMS (ESI)** for Chemical Formula: $C_{16}H_{17}N_2O_2S$ $(M+H)^+$ Calcd: 323.0825, Found: 323.0831.



2o

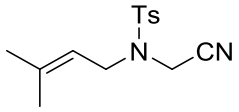
N-allyl-N-(cyanomethyl)-4-methylbenzenesulfonamide (2o): yellow liquid, 33.0 mg, (Yield: 66 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.75 (d, *J* = 8.4 Hz, 2H), 7.39 (d, *J* = 8.0 Hz, 2H), 5.73 (m, 1H), 5.35 (m, 2H), 4.21 (s, 2H), 3.83 (d, *J* = 7.6 Hz, 2H), 2.25 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 144.8, 134.2, 130.6, 130.1, 127.6, 121.8, 113.3, 50.2, 34.4, 21.6; **HRMS (ESI)** for Chemical Formula: $C_{12}H_{15}N_2O_2S$ $(M+H)^+$ Calcd: 251.0849; Found: 251.0855.



2p

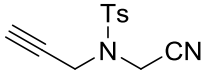
N-(cyanomethyl)-4-methyl-N-(pent-4-en-1-yl)benzenesulfonamide (2p): colorless liquid, 46.1 mg, (Yield: 83 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.74 (d, *J* = 8.4 Hz, 2H), 7.38 (d, *J* = 8.4 Hz, 2H), 5.78 (m, 1H), 5.04 (m, 2H), 4.26 (s, 2H), 3.21 (t, *J* = 7.4 Hz, 2H), 2.45 (s, 3H), 2.14 (dd, *J* = 7.2 Hz, 2H), 1.69 (m, 2H); **^{13}C NMR** (100 MHz,

$CDCl_3$): δ 144.6, 136.7, 134.3, 130.0, 127.5, 115.9, 113.6, 46.9, 35.1, 30.3, 26.5, 21.6; **HRMS (ESI)** for Chemical Formula: $C_{14}H_{19}N_2O_2S$ $(M+H)^+$ Calcd: 279.1162, Found: 279.1169.



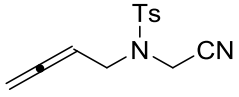
2q

N-(cyanomethyl)-4-methyl-N-(3-methylbut-2-en-1-yl)benzenesulfonamide (2q): colorless liquid, 48.4 mg, (Yield: 87 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.76 (d, *J* = 8.4 Hz, 2H), 7.39 (d, *J* = 8.0 Hz, 2H), 5.10 (m, 1H), 4.20 (s, 2H), 3.82 (d, *J* = 7.2 Hz, 2H), 2.46 (s, 3H), 1.76 (s, 3H), 1.69 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 144.5, 141.2, 134.3, 130.0, 127.6, 116.4, 113.8, 44.9, 34.0, 25.9, 21.6, 17.7; **HRMS (ESI)** for Chemical Formula: $C_{14}H_{19}N_2O_2S$ $(M+H)^+$ Calcd: 279.1162, Found: 279.1159.



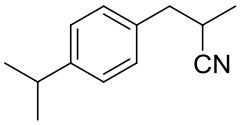
2r

N-(cyanomethyl)-4-methyl-N-(prop-2-yn-1-yl)benzenesulfonamide (2r)[18]**:** yellow liquid, 40.2 mg, (Yield: 81 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.74 (d, *J* = 8.4 Hz, 2H), 7.38 (d, *J* = 8.4Hz, 2H), 4.34 (s, 2H), 4.15 (d, *J* = 8.4 Hz, 2H), 2.46 (s, 3H), 2.30 (t, *J* = 2.4 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 145.1, 133.6, 130.1, 127.7, 113.3, 75.7, 74.7, 37.4, 34.8, 21.6; **MS (ESI, m/z):** Calculated for $[C_{12}H_{12}N_2O_2S]$ $(M+H)^+$ 271.1 found 271.1.



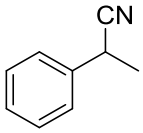
2s

N-(buta-2,3-dien-1-yl)-N-(cyanomethyl)-4-methylbenzenesulfonamide (2s):yellow liquid, 30.9 mg, (Yield: 59 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.75 (d, *J* = 8.4 Hz, 2H), 7.38 (d, *J* = 8.0 Hz, 2H), 5.04 (t, *J* = 6.8 Hz, 1H), 4.86 (m, 2H), 4.29 (s, 2H), 3.86 (m, 2H), 2.45 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 210.2, 144.8, 134.5, 130.1, 127.5, 113.5, 84.5, 77.2, 46.9, 34.5, 21.6; **MS (ESI, m/z):** Calculated for $[C_{13}H_{14}N_2O_2S]$ $(M+H)^+$ 263.0 found 263.0.



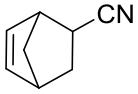
2t

3-(4-isopropylphenyl)-2-methylpropanenitrile (2t)[11]: colorless liquid, 29.2 mg, (Yield: 78 %).**^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.23 (d, *J* = 8.4 Hz, 2H), 7.19 (d, *J* = 8.0 Hz, 2H), 2.90 (m, 4H), 2.91 (t, *J* = 7.4 Hz, 2H), 1.36 (d, *J* = 6.8 Hz, 3H), 1.28 (d, *J* = 7.2 Hz, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ 147.7, 134.1, 128.9, 126.6, 122.7, 39.5, 33.7, 27.5, 23.9, 17.5; **MS (ESI, m/z):** Calculated for $[C_{13}H_{17}N]$ $(M+H)^+$ 188.1 found 188.0.



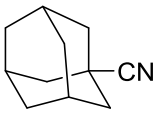
2u

2-phenylpropanenitrile (2u) [11]**:** colorless liquid, 23.6mg, (Yield: 90 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.43 (m, 5H), 3.94 (dd, *J* = 7.3 Hz, 1H), 1.67 (d, *J* = 7.2 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 137.0, 129.1, 128.0, 126.7, 121.5, 31.2, 21.4; **MS (ESI, m/z):** Calculated for $[C_9H_9N]$ $(M+H)^+$ 132.1 found 132.0.



2v

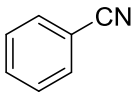
bicyclo[2.2.1]hept-5-ene-2-carbonitrile (2v)[19]**:**colorless liquid, 17.3 mg, (Yield:73 %).**^{1}H NMR** (400 MHz, $CDCl_3$): δ 6.34 (dd, *J* = 2.8 Hz, 1H), 6.21 (dd, *J* = 2.8 Hz, 1H), 3.24 (s, 1H), 3.03 (s, 1H), 2.87 (m, 1H), 2.17 (m, 1H), 1.54 (m, 1H), 152 (t, J =2.2 Hz, 1H), 1.36 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 138.9, 132.7, 123.2, 48.5, 45.7, 42.4, 32.5, 27.2; **MS (ESI, m/z):** Calculated for $[C_8H_9N]$ $(M+H)^+$ 120.1 found 120.0.



2w

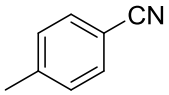
(3r,5r,7r)-adamantane-1-carbonitrile (2w)[20]**:** white solid, 30.3 mg (Yield: 94 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 2.07 (s, 9H), 1.73 (t, *J* = 13.8 Hz, 6H); **^{13}C NMR** (100

MHz, $CDCl_3$): δ 125.2, 39.8, 35.6, 30.1, 27.0; **MS (ESI, m/z):** Calculated for $[C_{11}H_{15}N]$ $(M+H)^+$ 162.1 found 162.1.



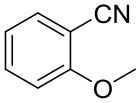
4a

benzonitrile (4a)[12]**:** colorless liquid, 16.0 mg, (Yield: 78 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.65 (m, 3H), 7.48 (d, *J* = 7.8 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 132.7, 132.0, 129.0, 118.7, 112.3; **MS (ESI, m/z):** Calculated for $[C_7H_5N]$ $(M+H)^+$ 104.0 found 104.1.



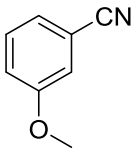
4b

4-methylbenzonitrile (4b)[12]**:** colorless liquid, 21.0 mg, (Yield: 90 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.55 (d, *J* = 8.0 Hz, 2H), 7.27 (t, *J* = 8.0 Hz, 2H), 2.42 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 143.7, 132.0, 129.8, 119.1, 109.3, 21.8; **MS (ESI, m/z):** Calculated for $[C_8H_7N]$ $(M+H)^+$ 118.1 found 118.1.



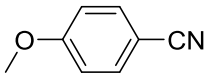
4c

2-methoxybenzonitrile (4c)[21]**:** yellow liquid, 26.0 mg (Yield: 98 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.54 (m, 2H), 7.00 (m, 2H), 3.93 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 161.2, 134.3, 133.7, 120.7, 116.4, 111.3, 101.7, 55.9; **MS (ESI, m/z):** Calculated for $[C_8H_7NO]$ $(M+H)^+$ 134.1 found 134.0.



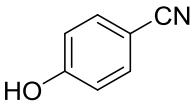
4d

3-methoxybenzonitrile (4d)[15]**:** colorless liquid, 23.9 mg, (Yield: 90 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.37 (m, 1H), 7.25 (m, 1H), 7.13 (m, 2H), 3.84 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 159.6, 130.3, 124.5, 119.1, 118.7, 116.8, 113.2, 55.5; **MS (ESI, m/z):** Calculated for $[C_8H_7NO]$ $(M+H)^+$ 134.1 found 134.0.



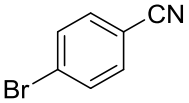
4e

4-methoxybenzonitrile (4e)[15]**:** white solid, 24.5 mg (Yield: 92 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.59 (d, *J* = 8.8 Hz, 2H), 6.96 (d, *J* = 8.8 Hz, 2H), 3.86 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 162.8, 133.9, 119.2, 114.7, 103.9, 55.5; **MS (ESI, m/z):** Calculated for $[C_8H_7NO]$ $(M+H)^+$ 134.1 found 134.1.



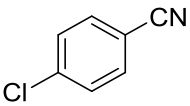
4f

4-hydroxybenzonitrile (4f)[19]**:** white solid, 18.3 mg (Yield: 77 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.56 (m, 2H), 6.94 (m, 2H), 6.83 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 160.3, 134.3, 119.2, 116.5, 102.9; **MS (ESI, m/z):** Calculated for $[C_7H_5NO]$ $(M-H)^+$ 118.0 found 117.9.



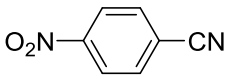
4g

4-bromobenzonitrile (4g)[12]**:** white solid, 23.9 mg (Yield: 66 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.66 (d, *J* = 8.4 Hz, 2H), 7.55 (d, *J* = 8.4Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 133.4, 132.6, 128.0, 118.1, 111.2; **MS (ESI, m/z):** Calculated for $[C_7H_4BrN]$ $(M+H)^+$ 182.0 found 181.9.



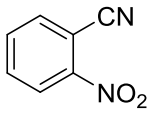
4h

4-chlorobenzonitrile (4h)[15]**:** white solid, 17.3 mg (Yield: 63 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.63 (d, *J* = 8.8 Hz, 2H), 7.49 (d, *J* = 8.4Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 139.6, 133.4, 129.7, 118.0, 110.7; **MS (ESI, m/z):** Calculated for $[C_7H_4ClN]$ $(M+H)^+$ 138.0 found 137.8.



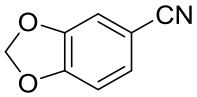
4i

4-nitrobenzonitrile (4i)[12]**:** white solid, 18.9 mg, (Yield: 64 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.38 (d, *J* = 8.8 Hz, 2H), 7.91 (d, *J* = 8.8 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 150.0, 133.5, 124.3, 118.3, 116.8; **MS (ESI, m/z):** Calculated for $[C_7H_4N_2O_2]$ $(M+H)^+$ 149.0 found 149.1.



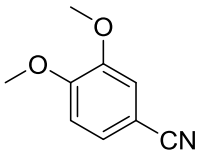
4j

2-nitrobenzonitrile (4j)[20]**:** white solid, 18.6 mg (Yield: 63 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.38 (m, 1H), 7.95 (m, 1H), 7.88 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 135.6, 134.3, 133.7, 125.5, 114.9, 108.1; **MS (ESI, m/z):** Calculated for $[C_7H_4N_2O_2]$ $(M+H)^+$ 149.0 found 148.9.



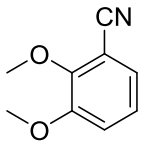
4k

benzo[d][1,3]dioxole-5-carbonitrile (4k)[15]**:** white solid, 26.1 mg (Yield: 89 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.22 (dd, *J* = 1.6 Hz, 1H), 7.04 (d, *J* = 1.6 Hz, 1H), 6.88 (d, *J* = 8.0 Hz, 1H), 6.07 (s, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 151.5, 148.0, 128.2, 118.8, 111.4, 109.1, 104.9, 102.2; **MS (ESI, m/z):** Calculated for $[C_8H_5NO_2]$ $(M+H)^+$ 148.0 found 147.9.



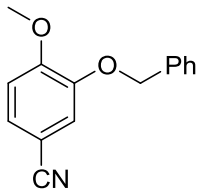
4l

3,4-dimethoxybenzonitrile(4l)[15]**:** white solid, 29.8 mg (Yield: 91 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.31 (dd, *J* = 8.2 Hz, 1H), 7.09 (d, *J* = 2.0 Hz, 1H), 6.93 (d, *J* = 8.4 Hz, 1H), 3.94 (s, 3H), 3.91 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 152.7, 149.0, 126.4, 119.2, 113.7, 111.1, 103.7, 56.0, 56.01; **MS (ESI, m/z):** Calculated for $[C_9H_9NO_2]$ $(M+H)^+$ 164.1 found 164.0.



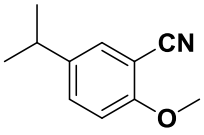
4m

2, 3-dimethoxybenzonitrile (4m)[22]**:** white solid, 30.3 mg (Yield: 93 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.12 (m, 3H), 4.02 (s, 3H), 3.89 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 152.6, 151.7, 124.4, 116.9, 116.2, 107.0, 61.6, 56.0; **MS (ESI, m/z):** Calculated for $[C_9H_9NO_2]$ $(M+H)^+$ 164.1 found 164.0.



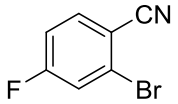
4n

2-(benzyloxy)-3-methoxybenzonitrile (4n)[23]**:** white solid, 44.4 mg (Yield: 93 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.43 (m, 6H), 7.10 (m, 2H), 5.14 (s, 2H), 3.92 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 153.5, 148.2, 135.8, 128.7, 128.2, 127.3, 126.8, 119.2, 116.4, 111.6, 103.7, 71.1, 56.1; **MS (ESI, m/z):** Calculated for $[C_{15}H_{13}NO_2]$ $(M+H)^+$ 240.1 found 240.0.



4o

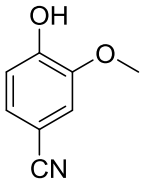
5-isopropyl-2-methoxybenzonitrile (4o): colorless liquid, 28.7 mg, (Yield: 82 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.38 (t, *J* = 5.0 Hz, 2H), 6.89 (t, *J* = 4.6 Hz, 1H), 3.90 (s, 3H), 2.87 (m, 1H), 1.23 (d, *J* = 6.8 Hz, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$)**:** δ 159.4, 141.4, 132.5, 131.3, 116.8, 111.2, 101.4, 56.0, 32.9, 23.8; **HRMS (ESI)** for Chemical Formula: $C_{11}H_{14}NO$ $(M+H)^+$ Calcd: 176.1070, Found: 176.1075.



4p

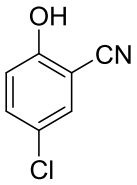
2-bromo-4-fluorobenzonitrile (4p)[24]**:** white solid, 28.6 mg (Yield: 72 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.71 (dd, *J* = 8.8Hz, 1H), 7.68 (dd, *J* = 8.0 Hz, 1H), 7.19 (m,

1H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 165.8 (d, *J* = 259 Hz), 136.0 (d, *J* = 9 Hz), 126.8 (d, *J* = 10 Hz), 121.3 (d, *J* = 25 Hz), 116.4, 115.8 (d, *J* = 22 Hz), 112.3 (d, *J* = 4 Hz); **^{19}F NMR** (376 MHz, $CDCl_3$): δ -100.4 (s). **MS (ESI, m/z):** Calculated for $[C_7H_3BrFN]$ $(M+H)^+$ 199.9 found 199.9.



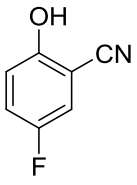
4q

4-hydroxy-3-methoxybenzonitrile (4q)[12]**:** white solid, 18.8 mg (Yield: 63 %). **^{1}H NMR** (400 MHz, DMSO-d_6): δ 10.26 (s, 1H), 7.35 (s, 1H), 7.28 (m, 1H), 6.91 (dd, *J* = 8.4 Hz, 1H), 3.80 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6): δ 151.4, 148.0, 126.5, 119.6, 116.1, 115.2, 100.9, 55.9; **MS (ESI, m/z):** Calculated for $[C_8H_7NO_2]$ $(M-H)^+$ 148.1 found 147.9.



4r

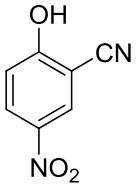
5-chloro-2-hydroxybenzonitrile (4r)[25]**:** yellow solid, 19.0 mg (Yield: 62 %). **^{1}H NMR** (400 MHz, DMSO-d_6): δ 11.40 (s, 1H), 7.75 (d, *J* =2.8 Hz, 1H), 7.55 (dd, *J* = 8.8 Hz, 1H), 7.03 (d, *J* = 1.2 Hz, 1H); **^{13}C NMR** (100 MHz, DMSO-d_6): δ 159.3, 134.7, 132.2, 122.6, 117.9, 115.7, 100.3; **MS (ESI, m/z):** Calculated for $[C_7H_4ClNO]$ $(M-H)^+$ 153.0 found 54.0.



4s

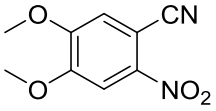
5-fluoro-2-hydroxybenzonitrile (4s)[26]**:** yellow solid, 12 mg (Yield: 44 %). **^{1}H NMR** (400 MHz, DMSO-d_6): δ 11.08 (s, 1H), 7.59 (dd, *J* = 8.6 Hz, 1H), 7.41 (m, 1H), 7.02(dd, *J* = 9.2 Hz, 1H); **^{13}C NMR** (100 MHz, DMSO-d_6): δ 157.2, 155.7 (d, *J* = 234

Hz), 122.5 (d, *J* = 24 Hz), 119.2 (d, *J* = 25 Hz), 117.8 (d, *J* = 8 Hz), 116.1, 99.3 (d, *J* = 10 Hz); **^{19}F NMR** (376 MHz, $CDCl_3$): δ -124.3 (s). **MS (ESI, m/z):** Calculated for $[C_7H_4FNO]$ $(M-H)^+$ 136.0 found 135.9.



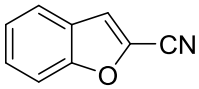
4t

2-hydroxy-5-nitrobenzonitrile (4t)[25]**:** yellow solid, 18.7 mg (Yield: 57 %). **^{1}H NMR** (400 MHz, DMSO-d_6): δ 8.58 (d, *J* = 2.8 Hz, 1H), δ 8.36 (dd, J = 9.2 Hz, 1H), 7.17 (d, *J* = 9.2 Hz, 1H); **^{13}C NMR** (100 MHz, DMSO-d_6): δ 165.7, 139.3, 130.3, 130.1, 116.8, 115.1, 99.7; **MS (ESI, m/z):** Calculated for $[C_7H_4N_2O_3]$ $(M-H)^+$ 163.0 found 162.9.



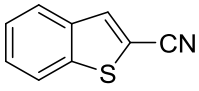
4u

4,5-dimethoxy-2-nitrobenzonitrile (4u)[27]**:** yellow solid, 22.1 mg (Yield: 53 %). **^{1}H NMR** (400 MHz, DMSO-d_6): δ 7.85 (s, 1H), 7.68 (s, 1H), 3.97 (s, 3H), 3.96 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6): δ 153.2, 151.8, 142.3, 116.4, 115.7, 108.4, 99.6, 57.1, 56.7; **MS (ESI, m/z):** Calculated for $[C_9H_8N_2O_4]$ $(M+H)^+$ 209.1 found 209.0.



4v

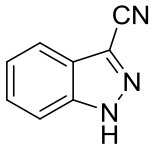
benzofuran-2-carbonitrile (4v)[12]**:** yellow liquid , 14.3 mg (Yield: 50 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.70 (d, *J* = 7.6 Hz, 1H), 7.50 (m, 3H), 7.35 (d, *J* = 1.2 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 155.7, 128.4, 127.3, 125.5, 124.6, 122.6, 118.4, 112.1, 111.8; **MS (ESI, m/z):** Calculated for $[C_9H_5NO]$ $(M+H)^+$ 144.0 found 143.9.



4w

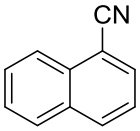
benzo[b]thiophene-2-carbonitrile (4w)[28]**:** yellow liquid, 18.4 mg, (Yield: 58 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.92 (m, 3H), 7.55 (m, 2H); **^{13}C NMR** (100 MHz,

$CDCl_3$): δ 141.3, 137.4, 135.0, 127.9, 125.7, 125.3, 122.4, 114.5, 109.7; **MS (ESI, m/z):** Calculated for $[C_9H_5NS]$ $(M+H)^+$ 160.0 found 160.0.



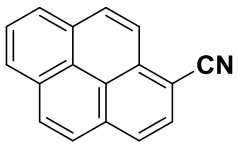
4x

1H-indazole-3-carbonitrile (4x)[29]**:** yellow solid, 20.3 mg (Yield: 71 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 11.86 (s, 1H), 7.58 (m, 4H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 140.0, 128.7, 124.3, 124.0, 119.6, 119.3, 113.6, 111.1; **MS (ESI, m/z):** Calculated for $[C_8H_5N_3]$ $(M+H)^+$ 144.0 found 144.0.



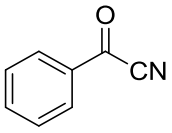
4y

1-naphthonitrile (4y)[20]**:** yellow liquid, 27.8 mg, (Yield: 91%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.25 (d, *J* = 8.4 Hz, 1H), 8.09 (d, *J* = 8.4 Hz, 1H), 7.92 (t, *J* = 6.8 Hz, 2H), 7.72 (t, *J* = 4.0 Hz, 1H), 7.65 (t, *J* = 14.0 Hz, 1H), 7.56 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 133.2, 132.9, 132.6, 132.3, 128.6, 128.5, 127.5, 125.1, 124.9, 117.8, 110.1; **MS (ESI, m/z):** Calculated for $[C_{11}H_7N]$ $(M+H)^+$ 154.0 found 154.0.



4z

pyrene-4-carbonitrile (4z)[30]**:** yellow solid, 39.9 mg (Yield: 88 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.24 (m, 3H), 8.09 (d, *J* = 8.0 Hz, 3H), 8.05 (t, *J* = 7.6 Hz, 1H),7.98 (d, *J* = 8.0 Hz, 1H), 7.92 (d, *J* = 8.8 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 133.8, 132.6, 130.5, 130.2, 130.1, 129.2, 126.8, 126.7, 124.1, 123.6, 123.1, 118.7, 105.3; **MS (ESI, m/z):** Calculated for $[C_{17}H_9N]$ $(M+H)^+$ 228.1 found 228.1.



4aa

Benzoyl cyanide (4aa)[31]**:** pale yellow solid, 19.3 mg (Yield: 74 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.14 (t, *J* = 8.4 Hz, 2H), 7.65 (t, *J* = 7.4 Hz, 1H), 7.51 (t, *J* = 8.0 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 167.9, 136.9, 133.4, 130.5, 129.5, 122.73; **MS (ESI, m/z):** Calculated for $[C_8H_5NO]$ $(M+H)^+$ 132.0 found 132.0.

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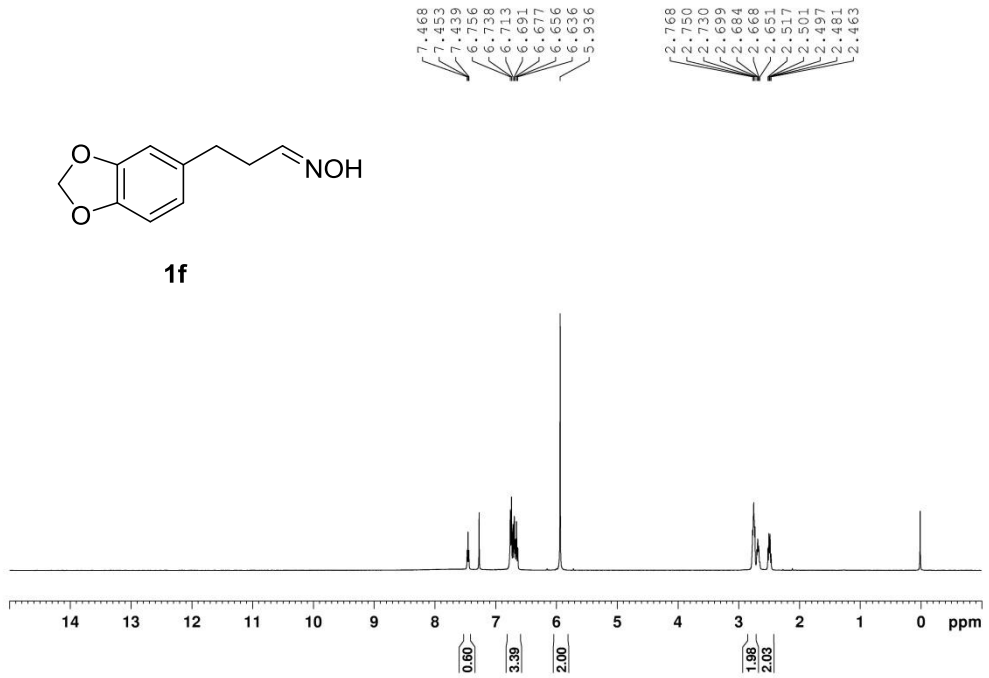
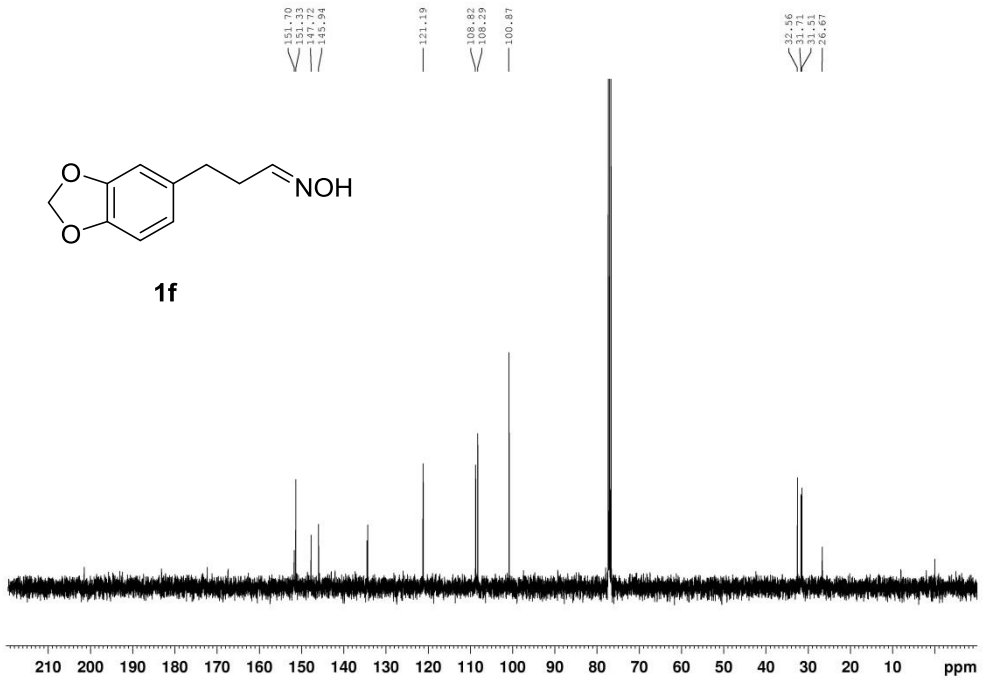
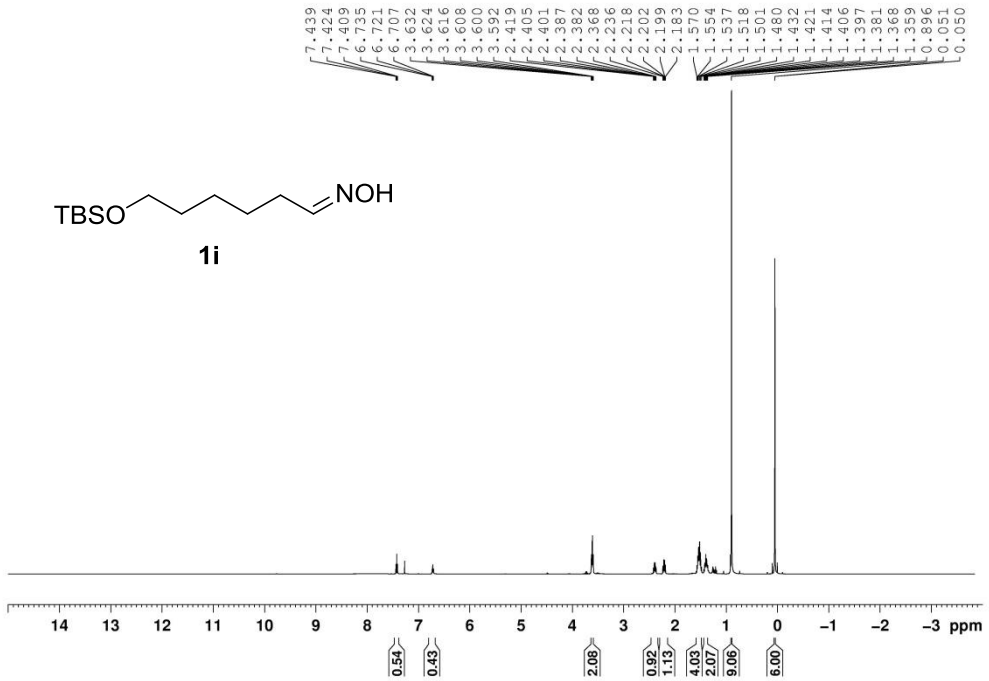
VIII. NMR Spectra

NMR Spectra of the Substrates



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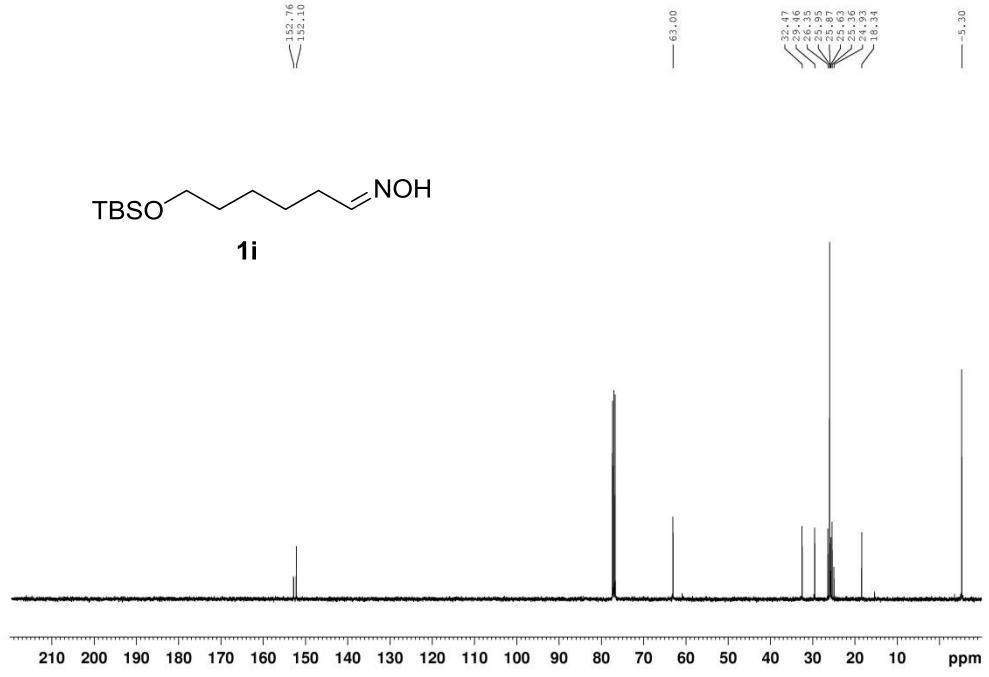
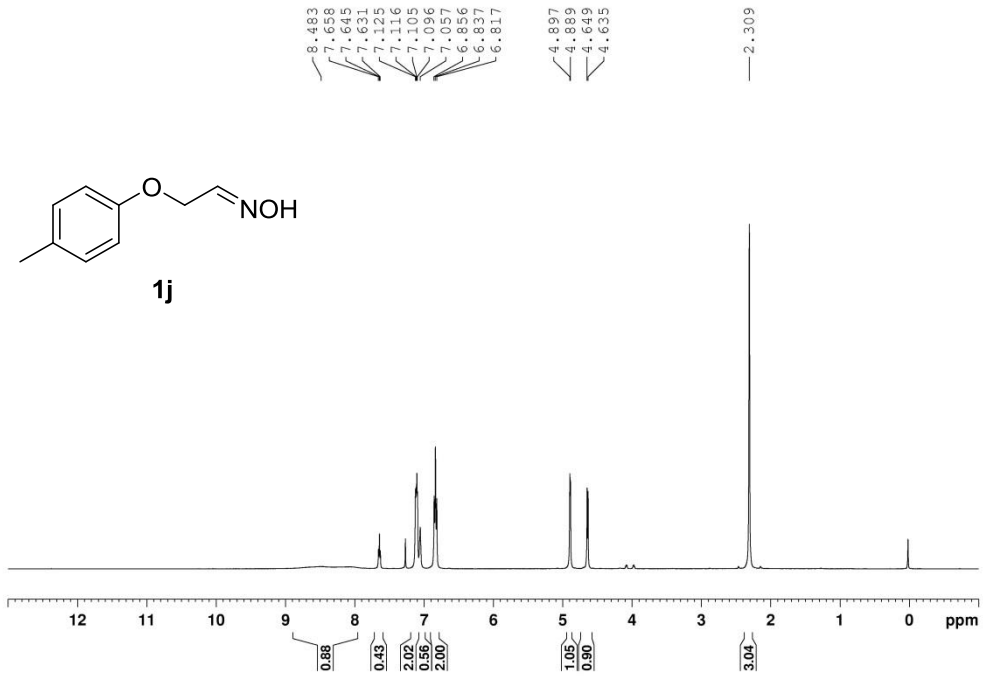
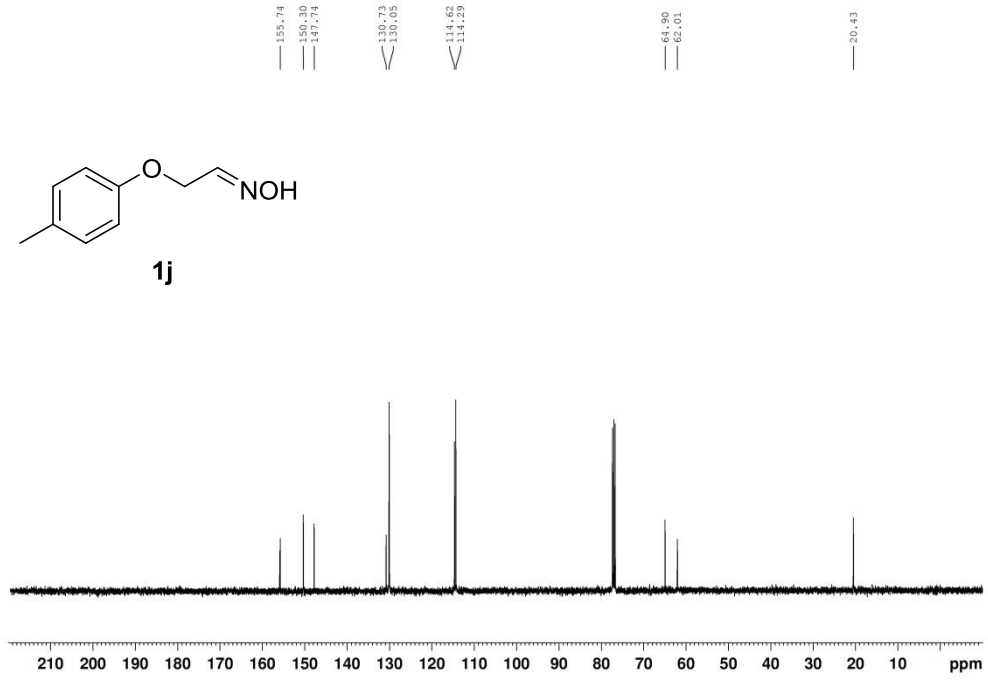
7.409
6.735
6.721
6.707
3.632
3.624
3.616
3.608
3.600
3.592
2.419
2.405
2.401
2.387
2.382
2.368
2.236
2.218
2.202
2.199
2.183
1.570
1.554
1.537
1.518
1.501
1.480
1.432
1.421
1.414
1.406
1.397
1.381
1.368
1.359
0.896
0.051
0.050
TBSO
NOH
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3 ppm
0.54
0.43
2.08
0.92
1.13
4.03
2.07
9.06
6.00

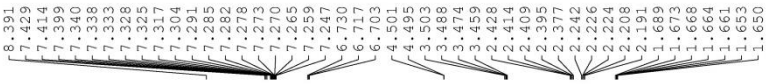
1i


152.76
152.10
63.00
32.47
29.46
26.35
25.95
25.87
25.63
25.36
14.93
-5.30
TBSO
NOH
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

1i


8.483
7.658
7.645
7.631
7.125
7.116
7.105
7.096
7.057
6.856
6.837
6.817
4.897
4.889
4.649
4.635
2.309
O
NOH
1j
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.88
0.43
2.02
0.56
2.00
1.05
0.90
3.04


155.74
150.30
147.74
130.73
130.05
114.62
114.29
64.90
62.01
20.43
O
NOH
1j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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7.429
7.414
7.399
7.340
7.338
7.333
7.328
7.325
7.317
7.304
7.291
7.285
7.282
7.278
7.273
7.270
7.265
7.259
7.247
6.730
6.717
6.703
4.501
4.495
3.503
3.488
3.474
3.459
2.428
2.414
2.409
2.395
2.377
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1.668
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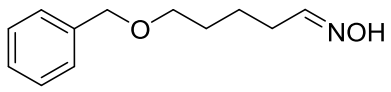
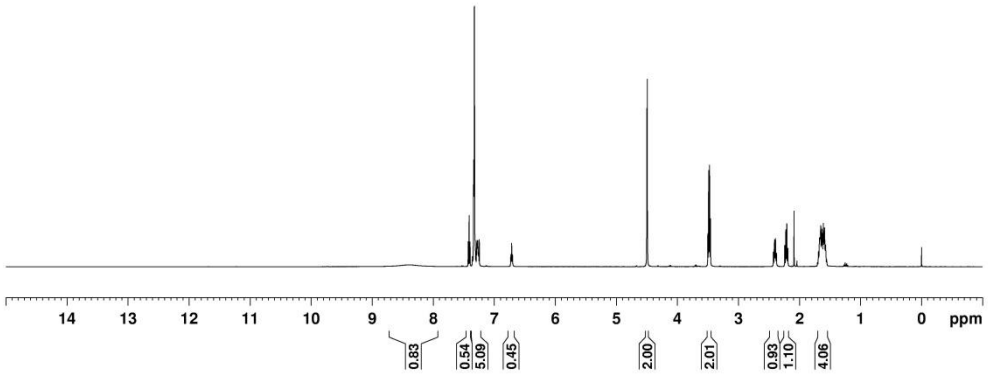
1.661
1.653
1.650


O
NOH

1k


14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
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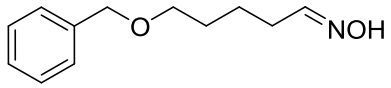
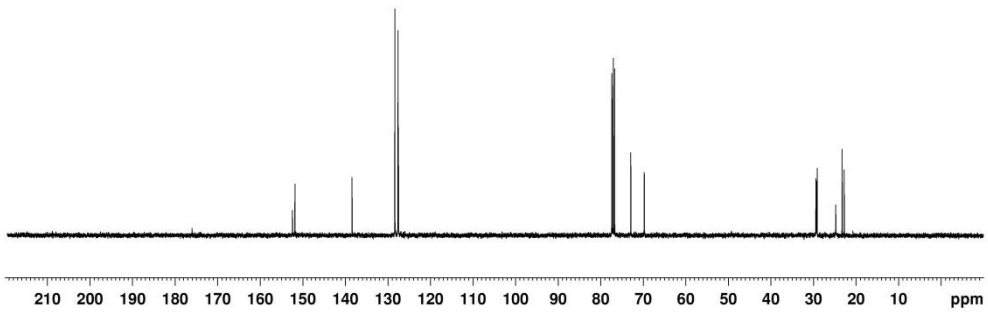
0.54
5.09
0.45
2.00
2.01
0.93
1.10
4.06


152.39
151.80
138.39
128.32
127.59
127.50
72.86
69.71
29.35
29.21
29.06
24.70
23.21
22.72


O
NOH

1k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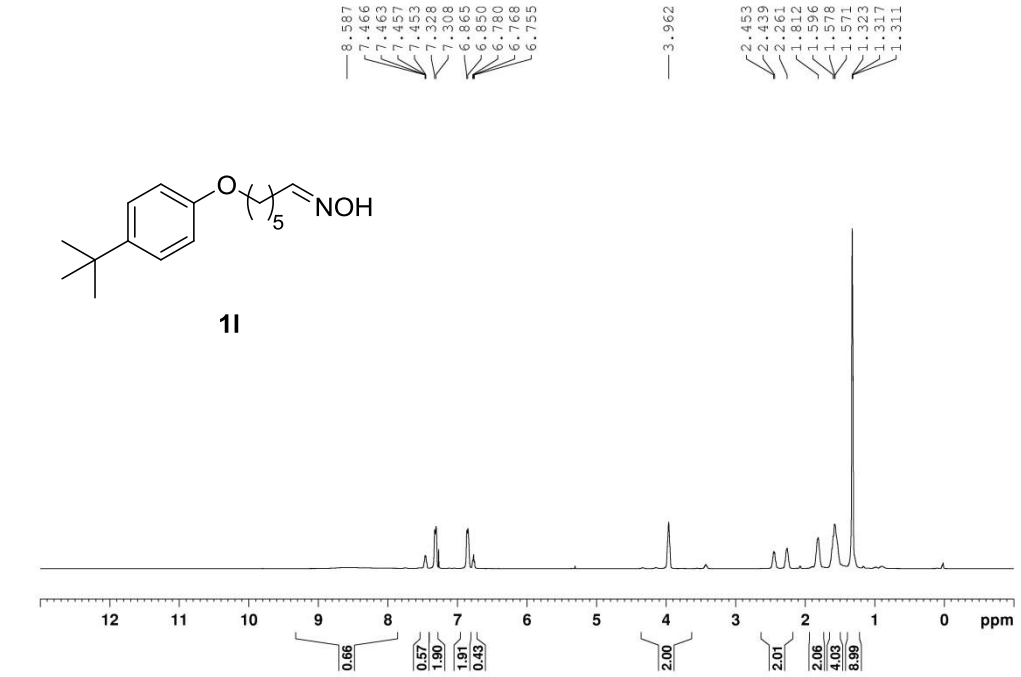
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7.463
7.457
7.453
7.328
7.308
6.865
6.850
6.780
6.768
6.755
3.962
2.453
2.439
2.261
1.812
1.596
1.578
1.571
1.323
1.317
1.311
O
5
NOH
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
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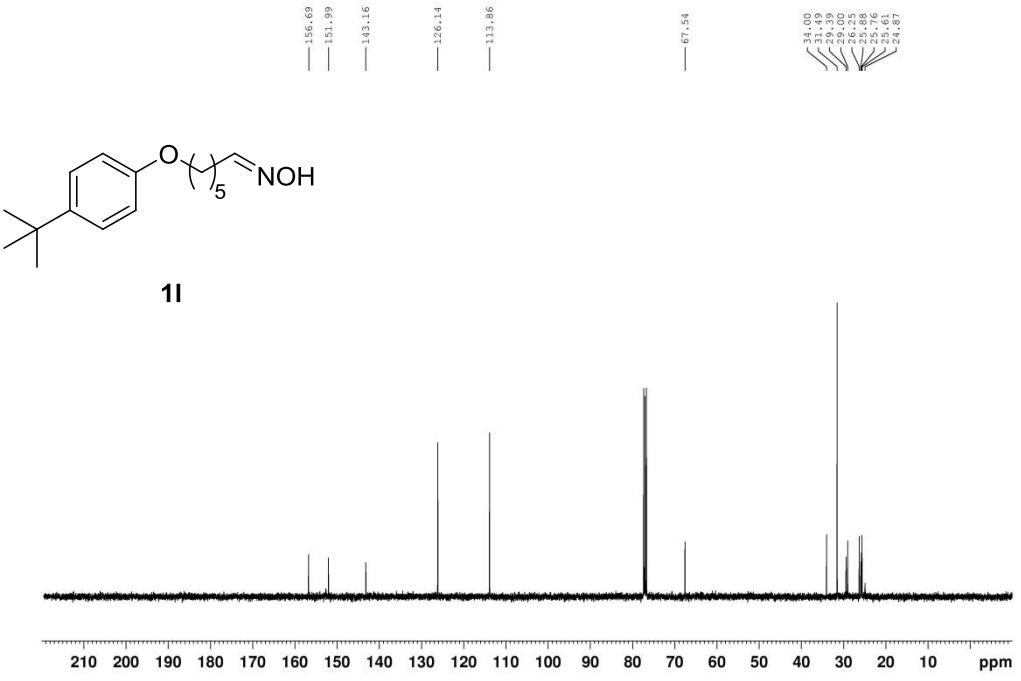
2.00
2.01
2.06
4.03
8.99

1l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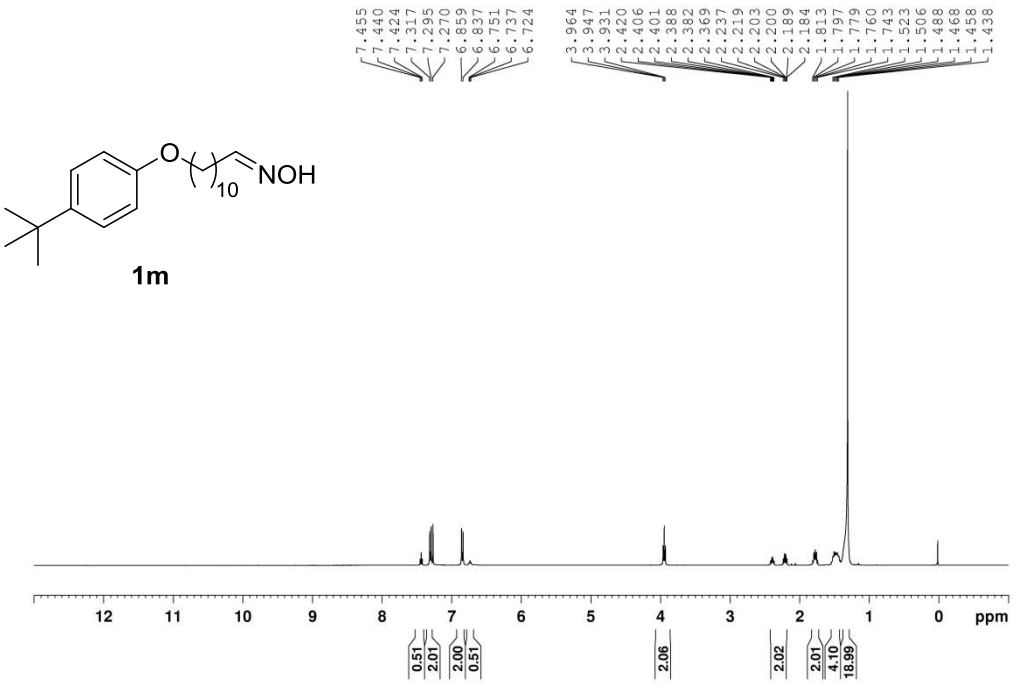
126.14
113.86
67.54
34.00
31.49
29.39
29.00
26.55
25.88
25.76
25.61
24.87
O
5
NOH
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

1l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7.424
7.317
7.295
7.270
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6.837
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6.737
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3.964
3.947
3.931
2.420
2.406
2.401
2.388
2.382
2.369
2.237
2.219
2.203
2.200
2.189
2.184
1.813
1.797
1.779
1.760
1.743
1.523
1.506
1.488
1.468
1.458
1.438
O
10
NOH
1m
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
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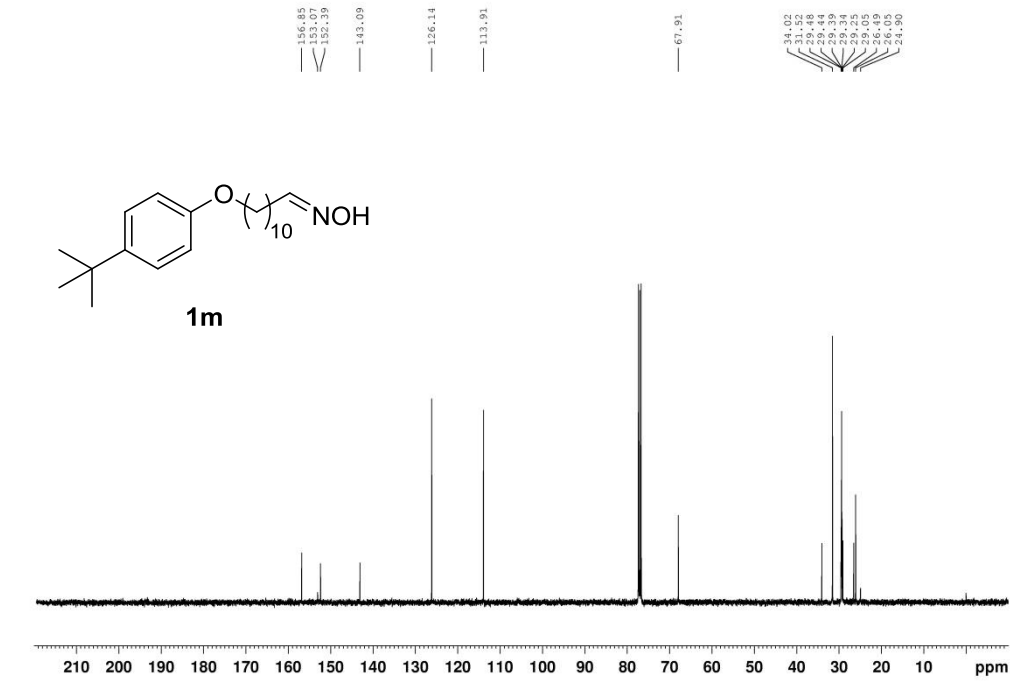
2.06
2.02
2.01
4.10
18.99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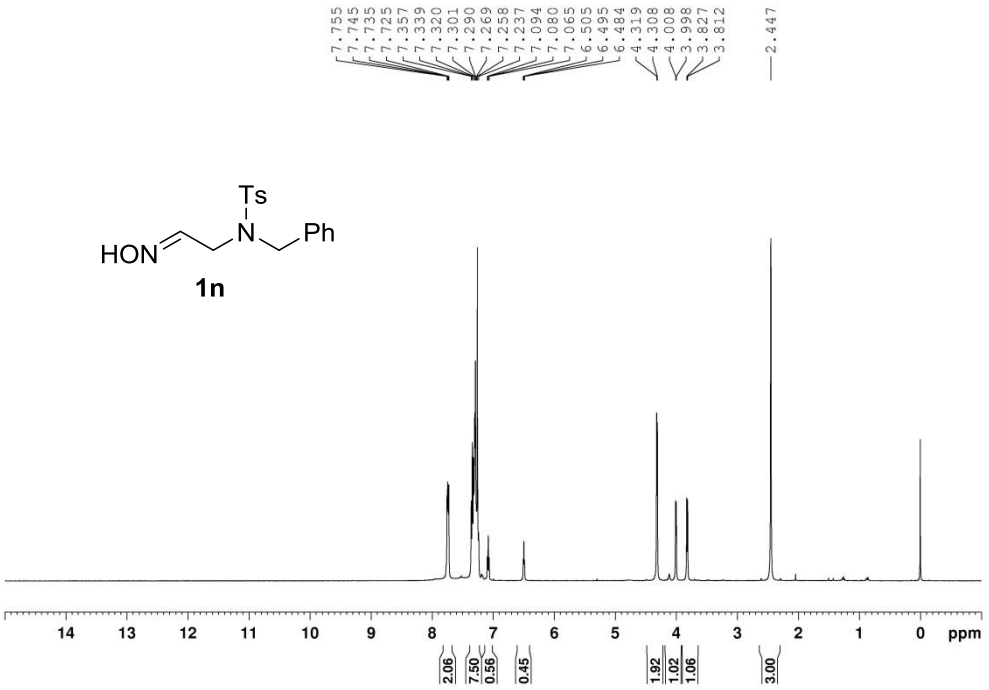
143.09
126.14
113.91
67.91
34.02
31.52
29.48
29.44
29.39
29.34
29.25
29.05
26.49
26.05
24.90
O
10
NOH
1m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.755
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7.339
7.320
7.301
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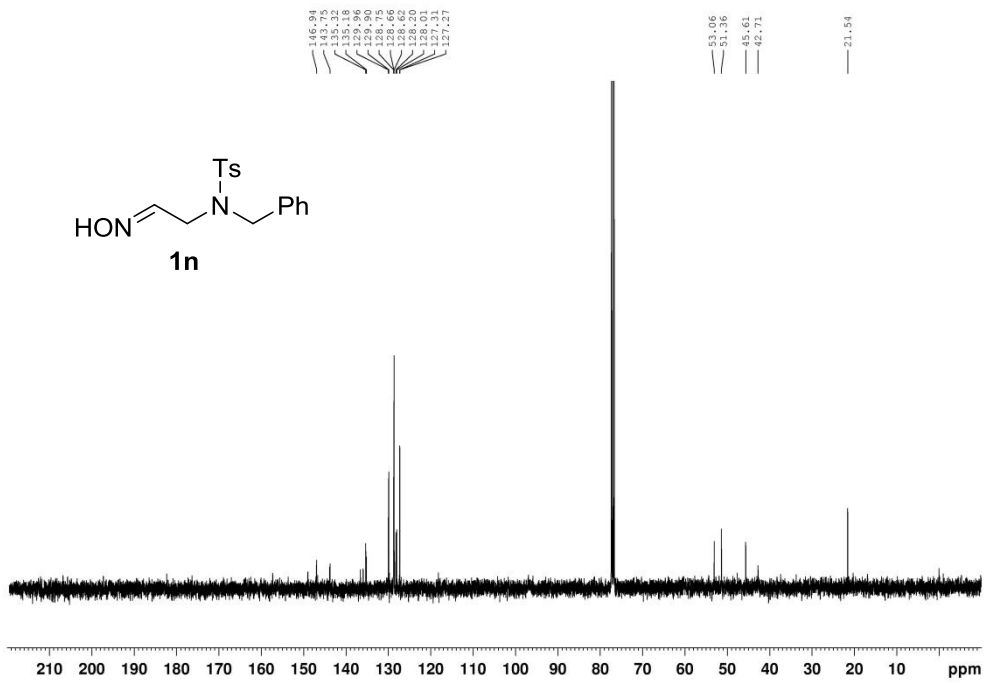
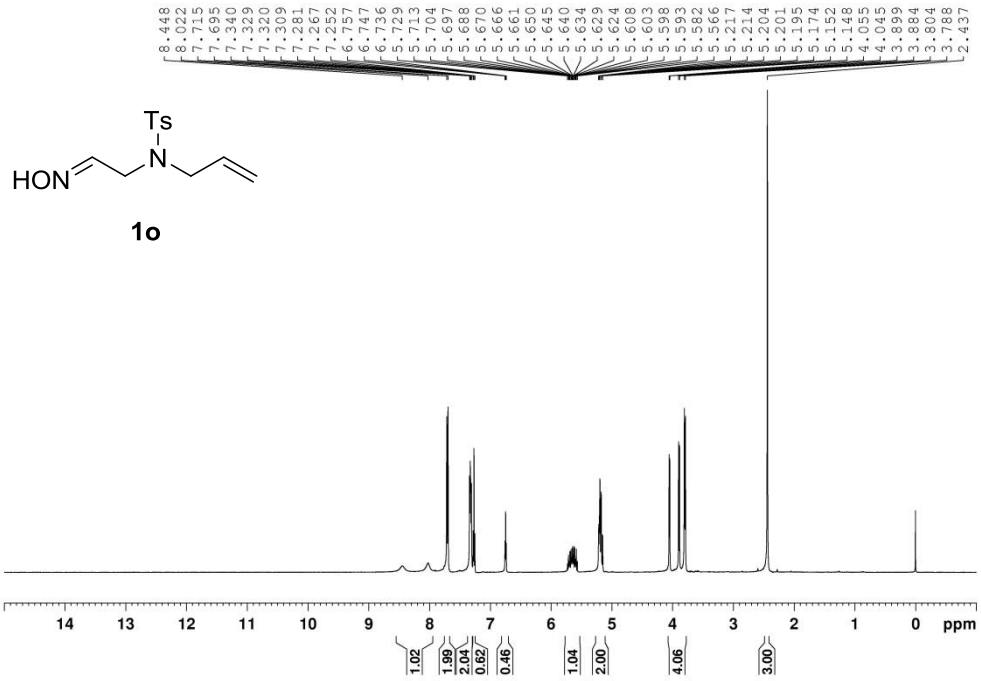
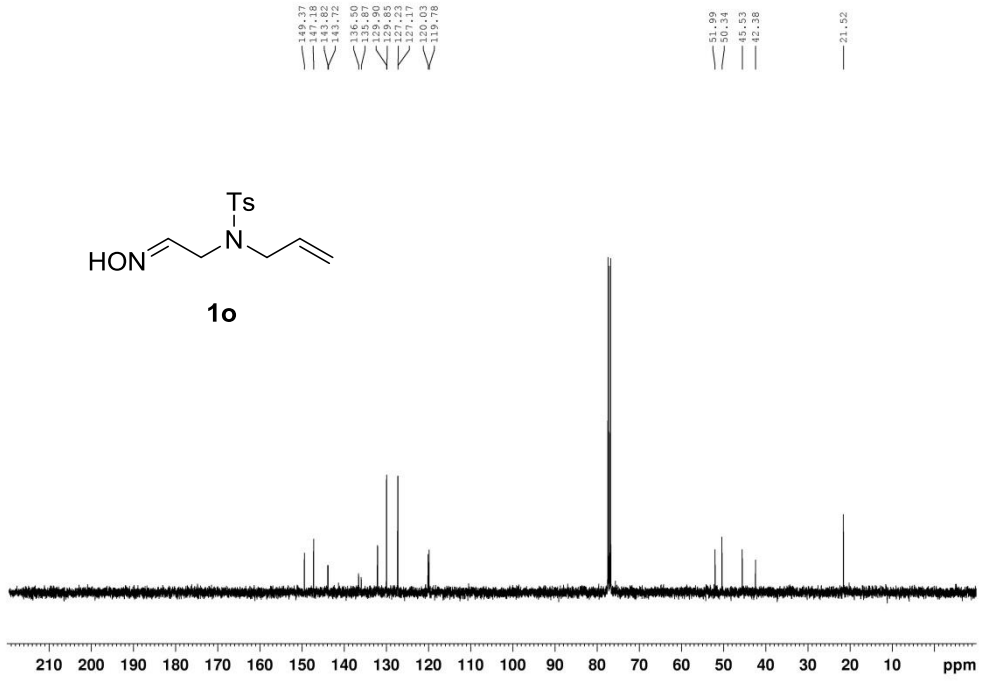
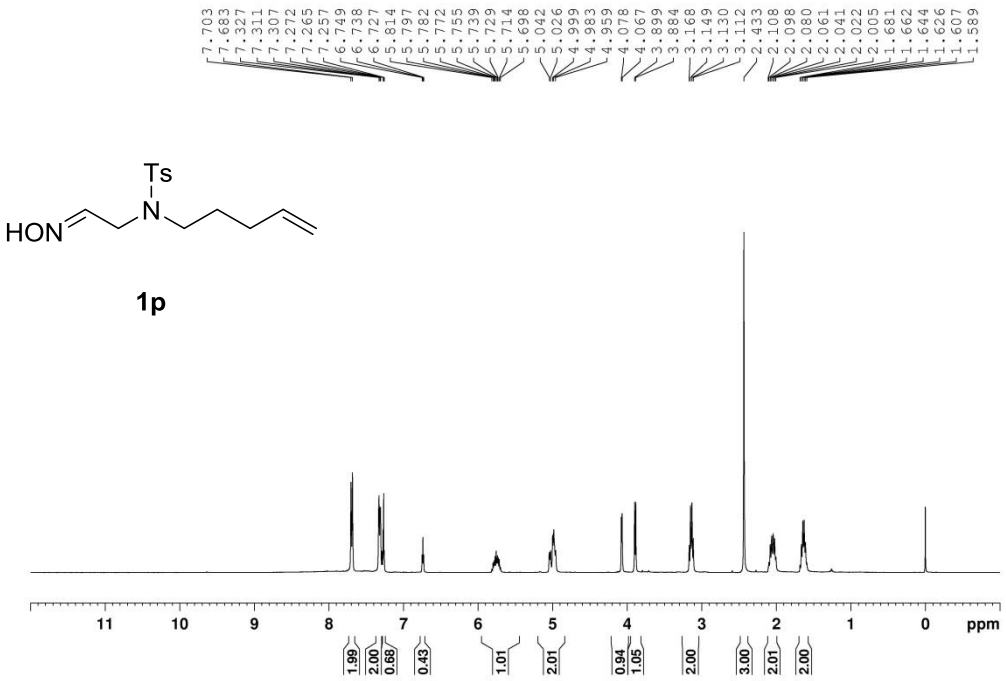
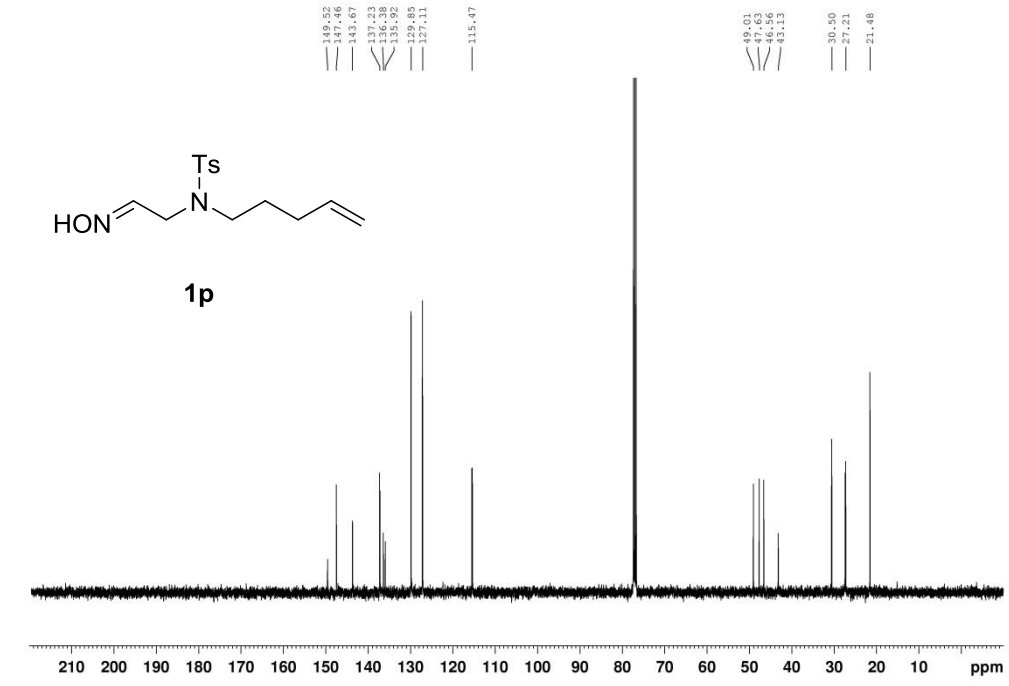
7.269
7.258
7.237
7.094
7.080
7.065
6.505
6.495
6.484
4.319
4.308
4.008
3.998
3.827
3.812
2.447
Ts
N
Ph
HON
1n
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.06
7.50
0.56
0.45
1.92
1.02
1.06
3.00

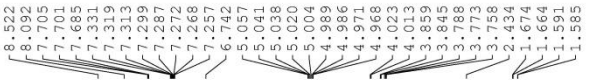

146.94
143.75
135.32
135.18
129.96
129.90
128.75
128.66
128.62
128.00
128.01
127.31
127.27
53.06
51.36
45.61
42.71
21.54
Ts
N
Ph
HON
1n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

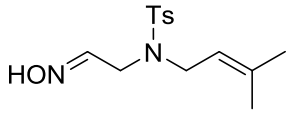

8.448
8.022
7.715
7.695
7.340
7.329
7.320
7.309
7.281
7.267
7.252
6.757
6.747
6.736
5.729
5.713
5.704
5.697
5.688
5.670
5.666
5.661
5.650
5.645
5.640
5.634
5.629
5.624
5.608
5.603
5.598
5.593
5.582
5.566
5.217
5.214
5.204
5.201
5.195
5.174
5.152
5.148
4.055
4.045
3.899
3.884
3.804
3.788
2.437
Ts
N
HON
1o
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.02 1.99 2.04 0.62 0.46 1.04 2.00 4.06 3.00


149.37
147.18
143.82
143.72
136.50
135.87
129.90
129.85
127.23
127.17
120.03
119.78
51.99
50.34
45.53
42.38
21.52
Ts
N
HON
1o
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

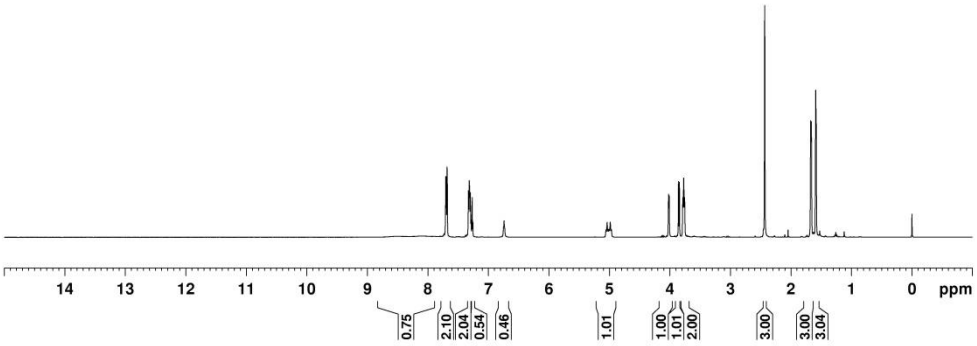

7.703
7.683
7.327
7.311
7.307
7.272
7.265
7.257
6.749
6.738
6.727
5.814
5.797
5.782
5.772
5.755
5.739
5.729
5.714
5.698
5.042
5.026
4.999
4.983
4.959
4.078
4.067
3.899
3.884
3.168
3.149
3.130
3.112
2.433
2.108
2.098
2.080
2.061
2.041
2.022
2.005
1.681
1.662
1.644
1.626
1.607
1.589
Ts
N
HON
1p
11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.99 2.00 0.68 0.43 1.01 2.01 0.94 1.05 2.00 3.00 2.01 2.00

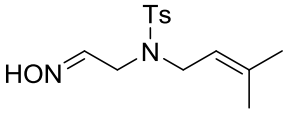

149.52
147.46
143.67
137.23
136.38
135.92
129.85
127.11
115.47
49.01
47.63
46.56
43.13
30.50
27.21
21.48
Ts
N
HON
1p
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.522
8.092
7.705
7.701
7.685
7.331
7.319
7.313
7.299
7.287
7.272
7.268
7.257
6.742
5.057
5.041
5.038
5.020
5.004
4.989
4.986
4.971
4.968
4.023
4.013
3.859
3.845
3.788
3.773
3.758
2.434
1.674
1.664
1.591
1.585


Ts
N
HON

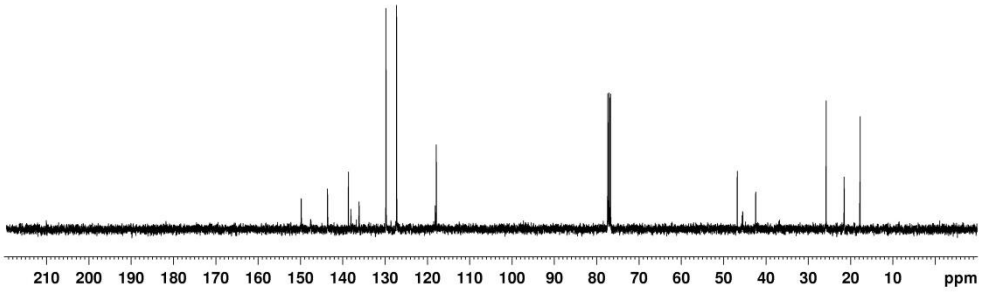
1q

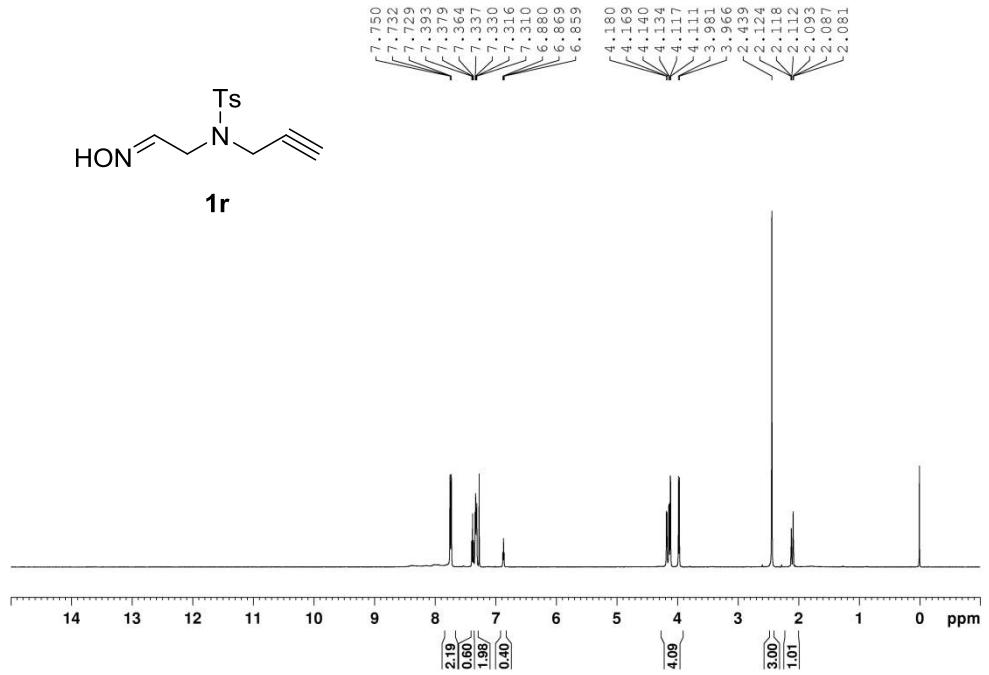

14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.75
2.10
2.04
0.54
0.46
1.01
1.00
1.01
2.00
3.00
3.00
3.04

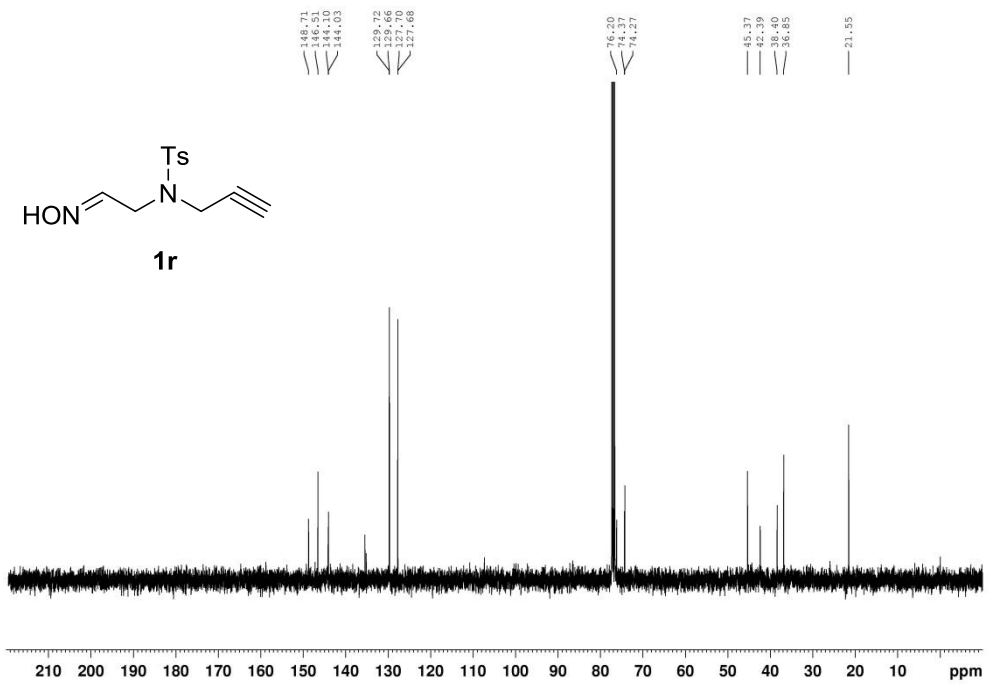

Ts
N
HON

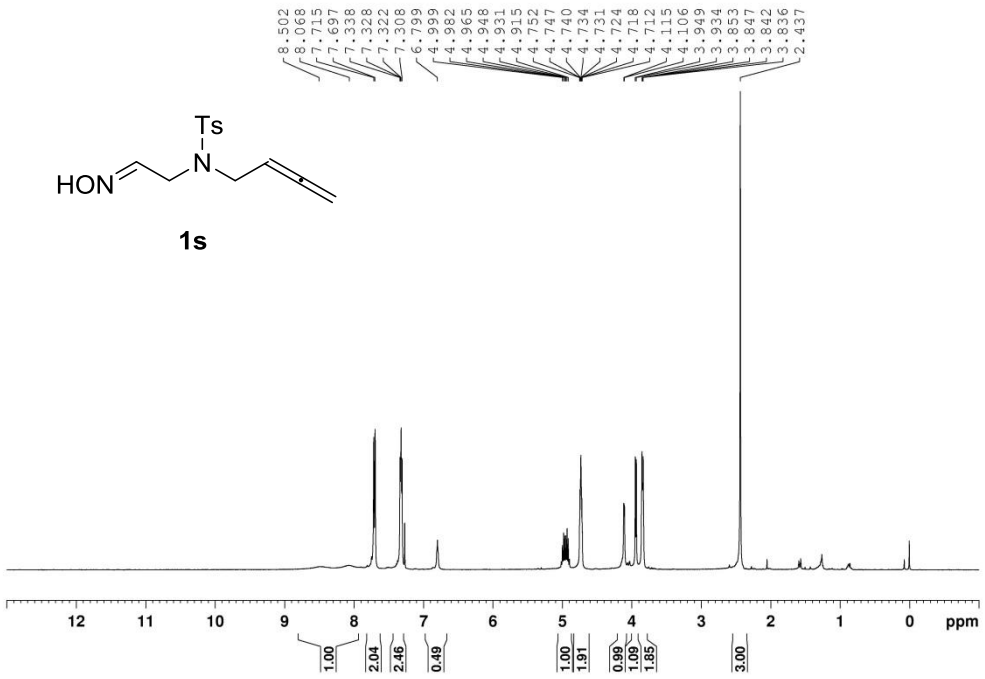
1q

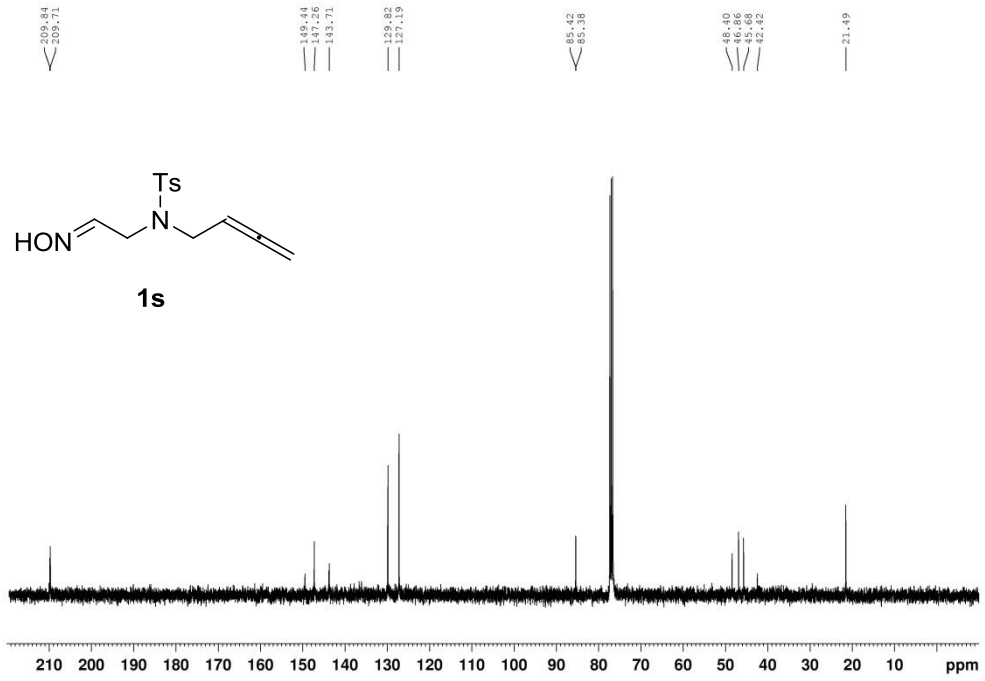

149.79
143.57
138.63
134.54
136.10
129.77
127.25
117.86
46.72
45.57
45.42
42.36
25.72
21.47
17.68

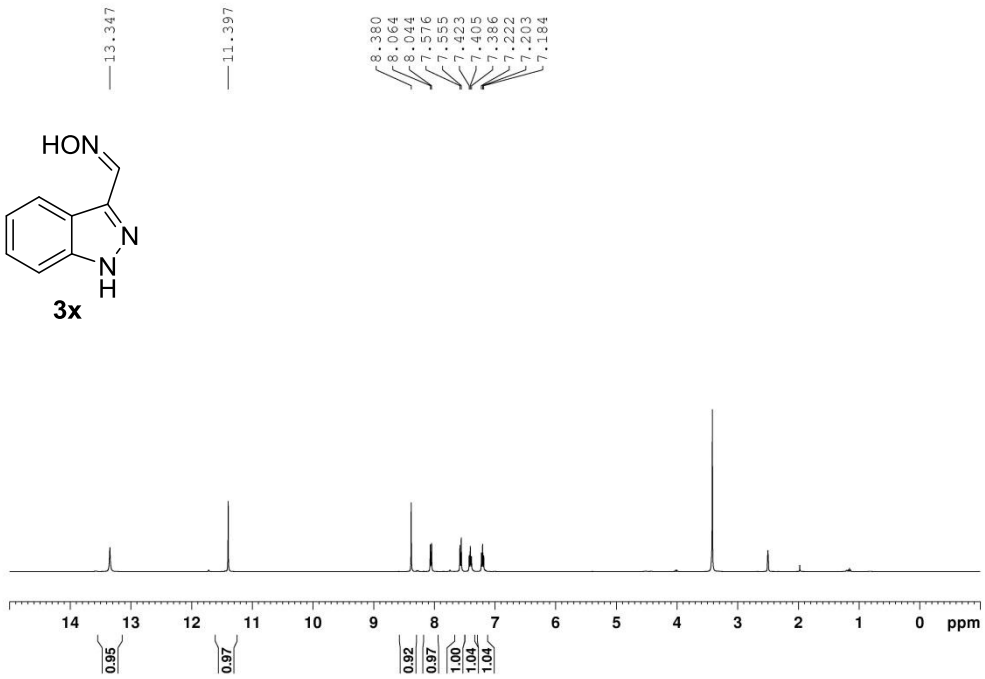

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

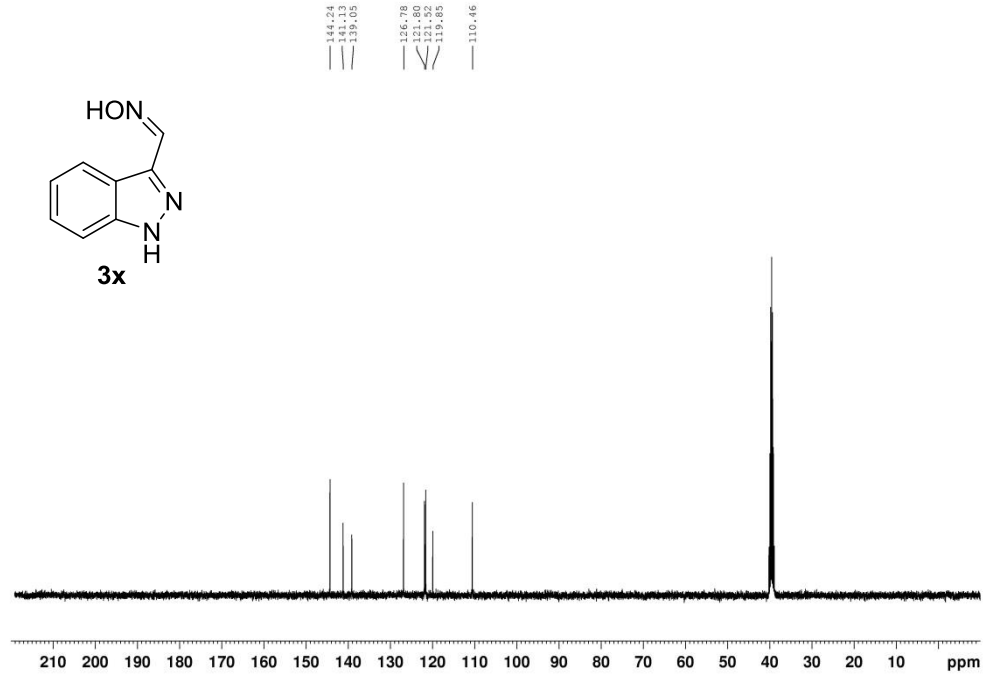

7.750
7.732
7.729
7.393
7.379
7.364
7.337
7.330
7.316
7.310
6.880
6.869
6.859
4.180
4.169
4.140
4.134
4.117
4.111
3.981
3.966
2.439
2.124
2.118
2.112
2.093
2.087
2.081
Ts
N
HON
1r
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.19
0.60
1.98
0.40
4.09
3.00
1.01


148.71
146.51
144.10
144.03
129.72
129.66
127.70
127.68
76.20
74.37
74.27
45.37
42.39
38.40
36.85
21.55
Ts
N
HON
1r
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

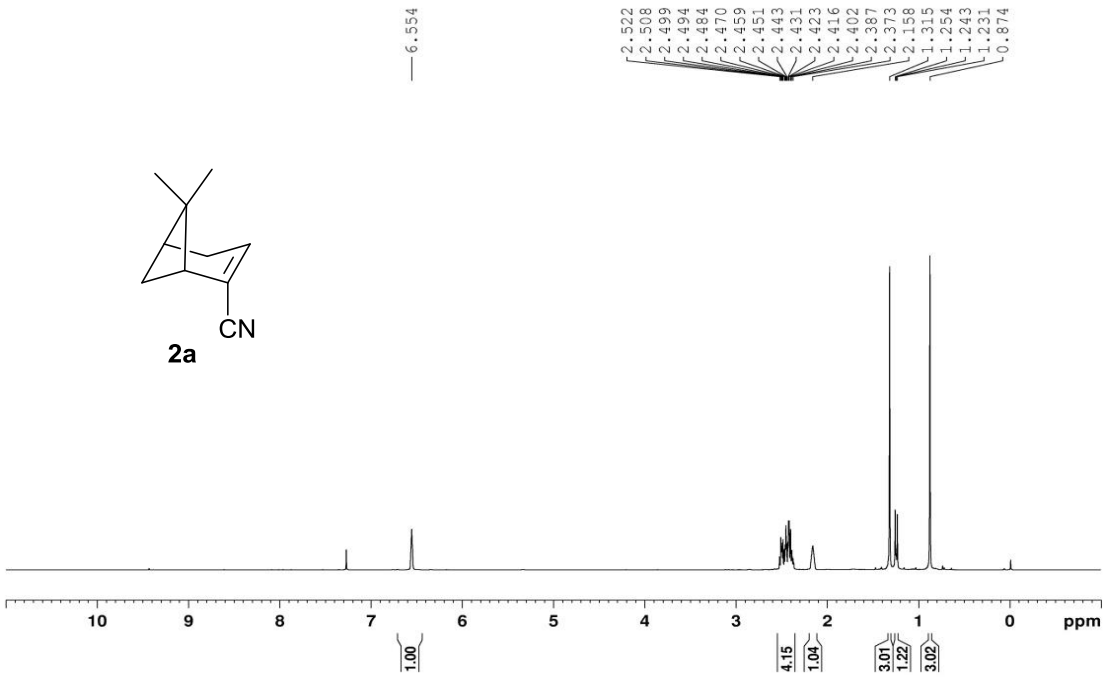

8.502
8.068
7.715
7.697
7.338
7.328
7.322
7.308
6.799
4.999
4.982
4.965
4.948
4.931
4.915
4.752
4.747
4.740
4.734
4.731
4.724
4.718
4.712
4.115
4.106
3.949
3.934
3.853
3.847
3.842
3.836
2.437
Ts
N
HON
1s
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00 2.04 2.46 0.49 1.00 1.91 0.99 1.09 1.85 3.00

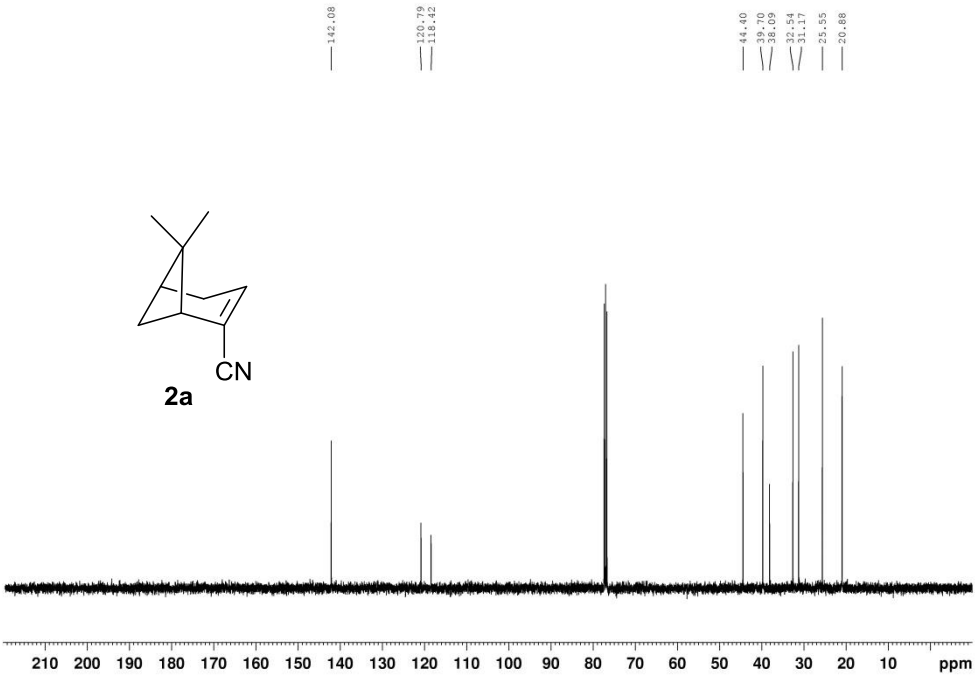

209.84
209.71
149.44
147.46
143.71
129.82
127.19
85.42
85.38
48.40
46.86
45.68
42.42
21.49
Ts
N
HON
1s
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


13.347
11.397
8.380
8.064
8.044
7.576
7.555
7.423
7.405
7.386
7.222
7.203
7.184
HON
N
N
H
3x
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.95
0.97
0.92
0.97
1.00
1.04
1.04

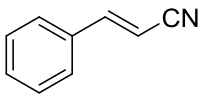

144.04
141.13
139.05
126.78
121.80
121.32
119.86
110.46
HON
N
N
H
3x
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

NMR Spectra of the Products

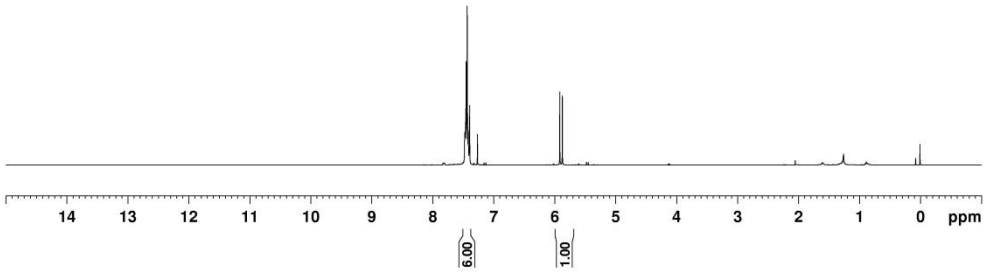


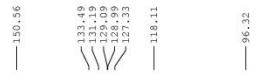


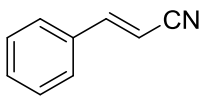

7.479
7.475
7.471
7.466
7.460
7.454
7.443
7.438
7.428
7.422
7.418
7.404
7.396
5.918
5.876


CN

2b

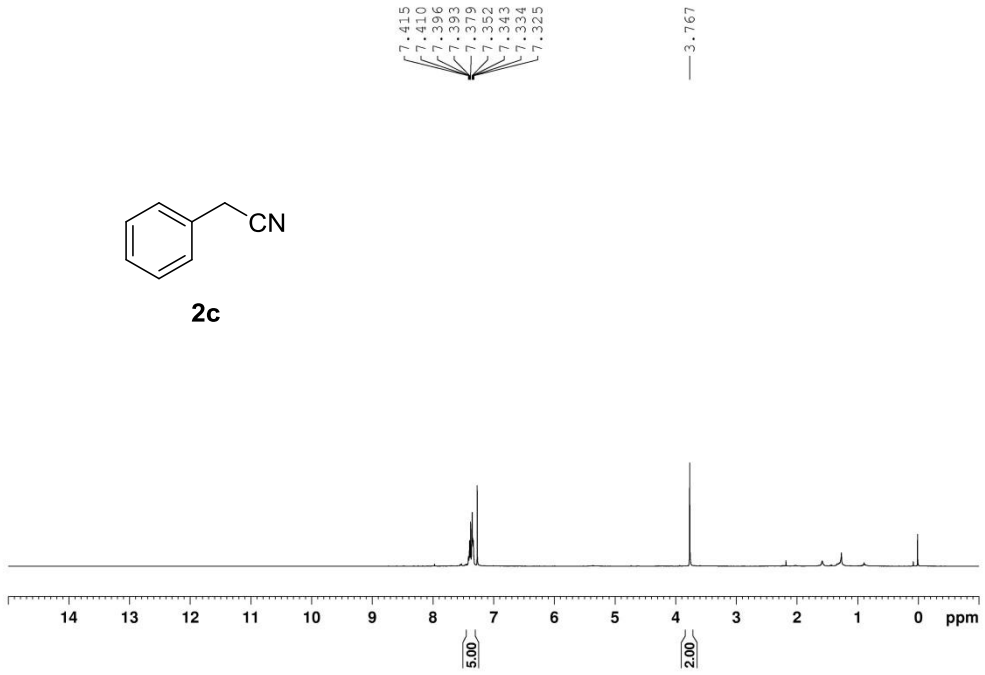

14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
6.00
1.00

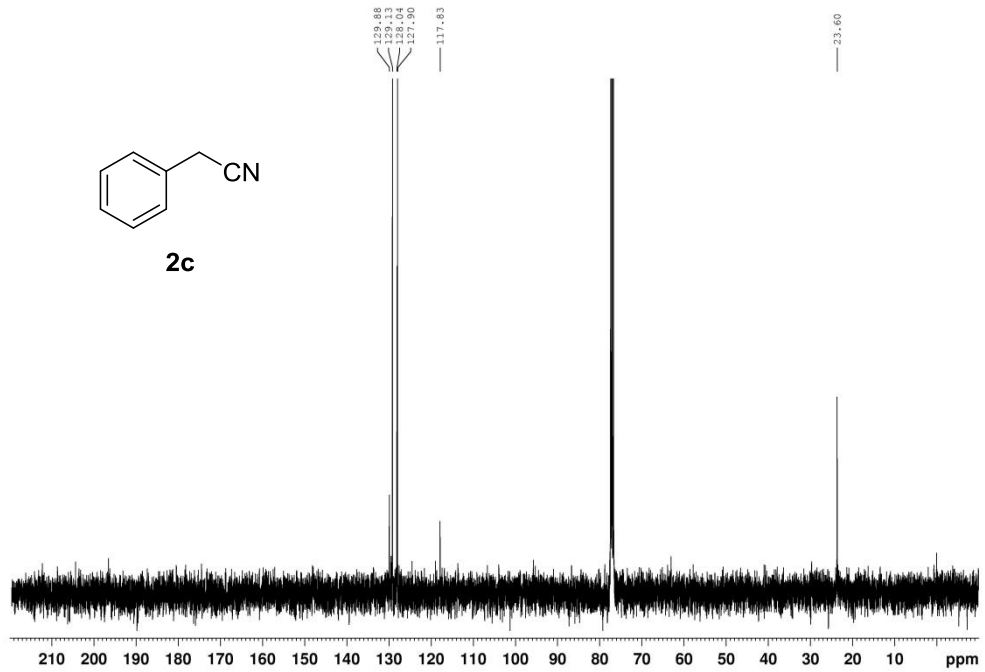

150.56
133.49
131.19
129.09
128.99
127.33
118.11
96.32

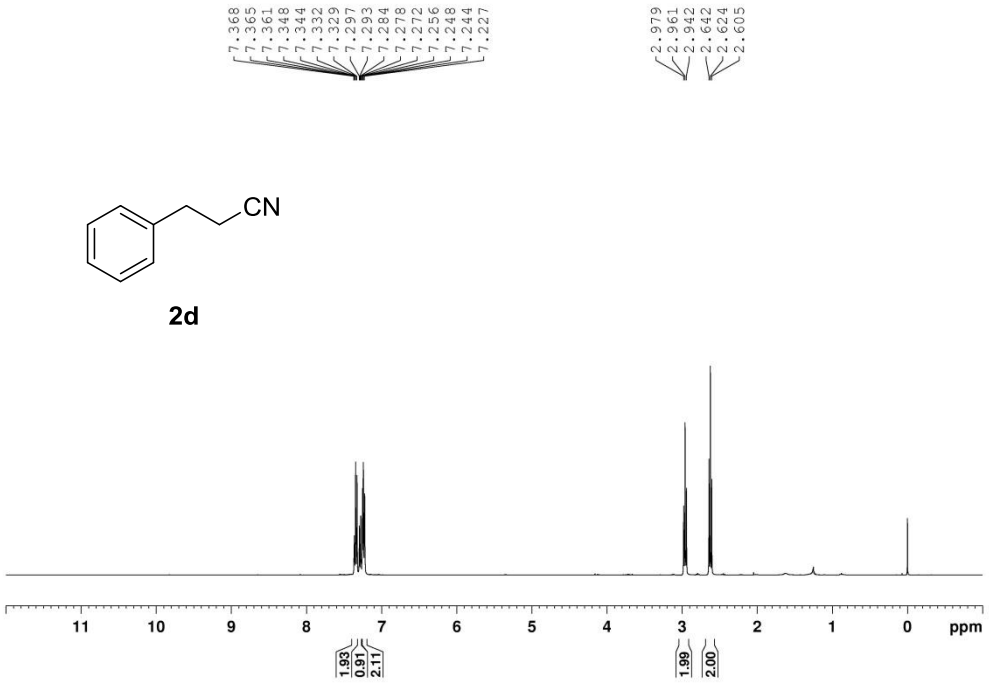

CN

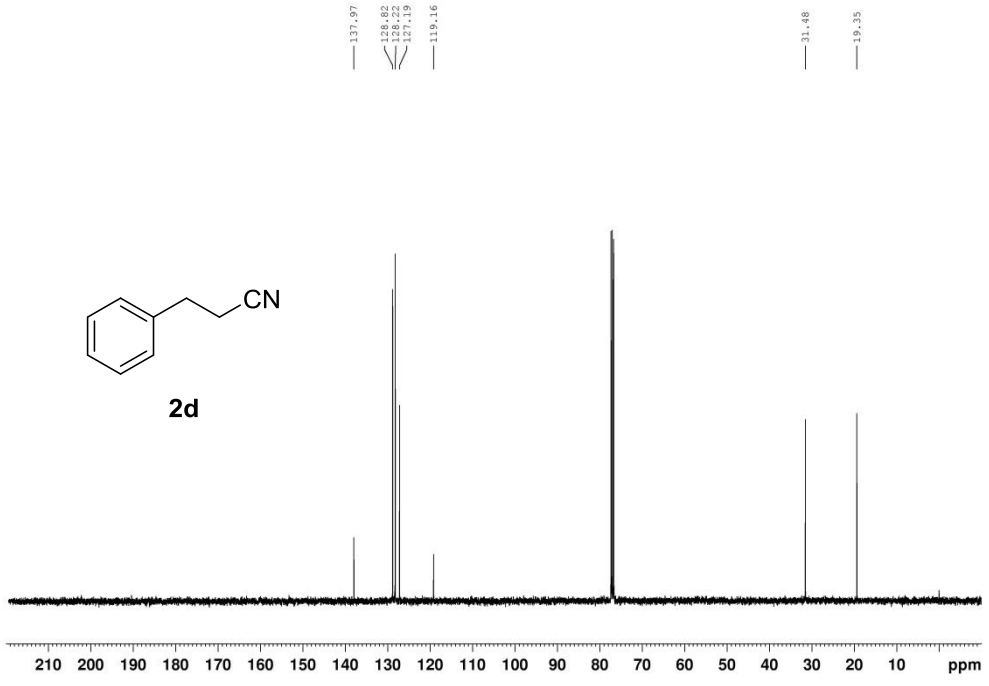
2b

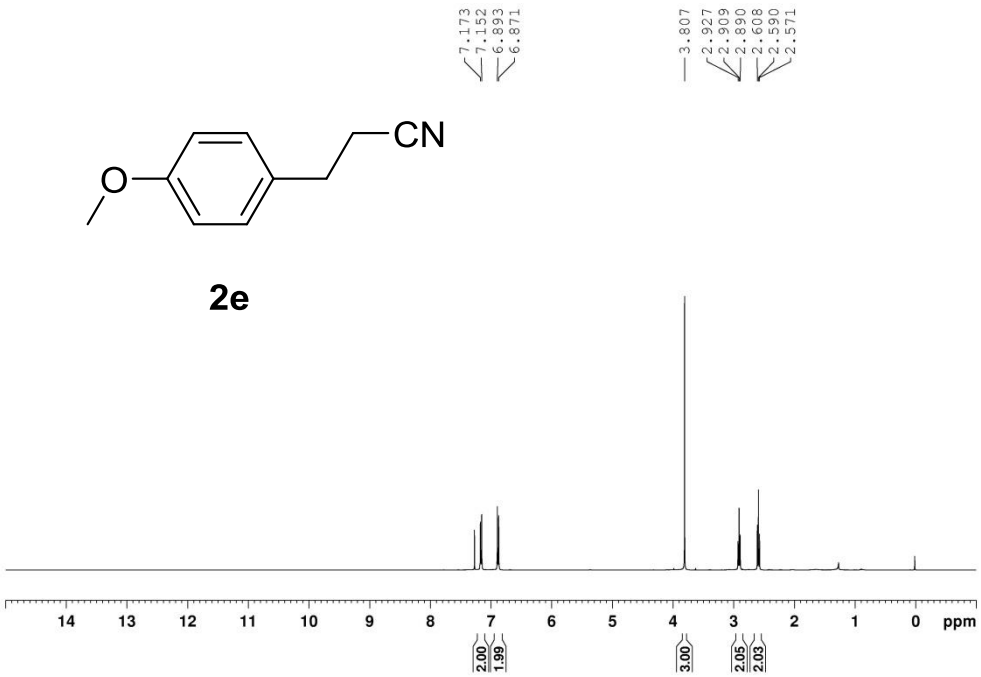
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

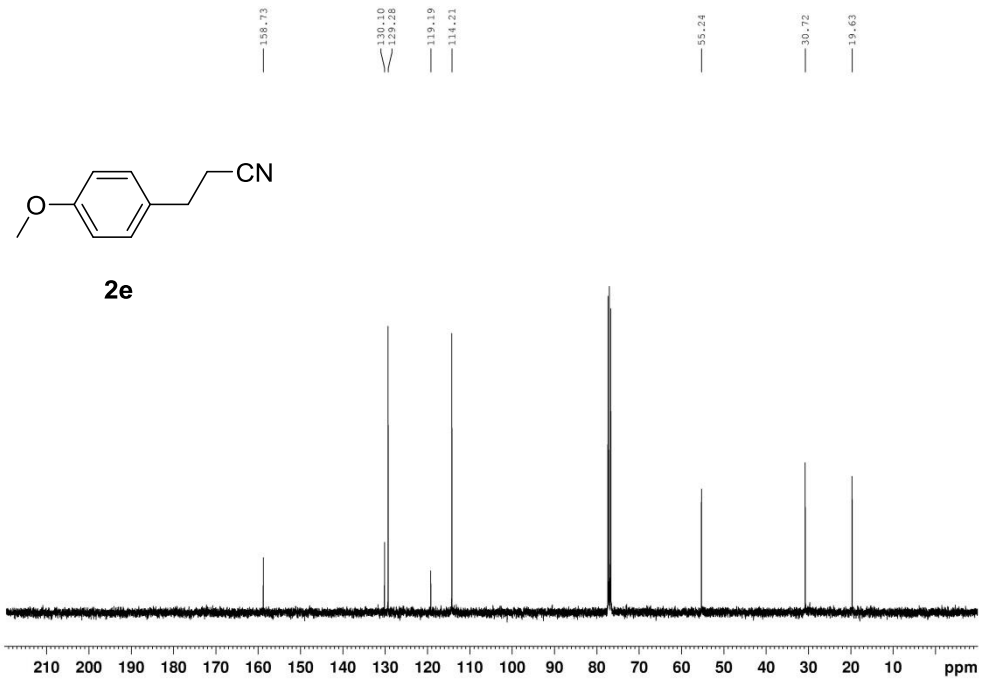

7.415
7.410
7.396
7.393
7.379
7.352
7.343
7.334
7.325
3.767
CN
2c
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
5.00
2.00

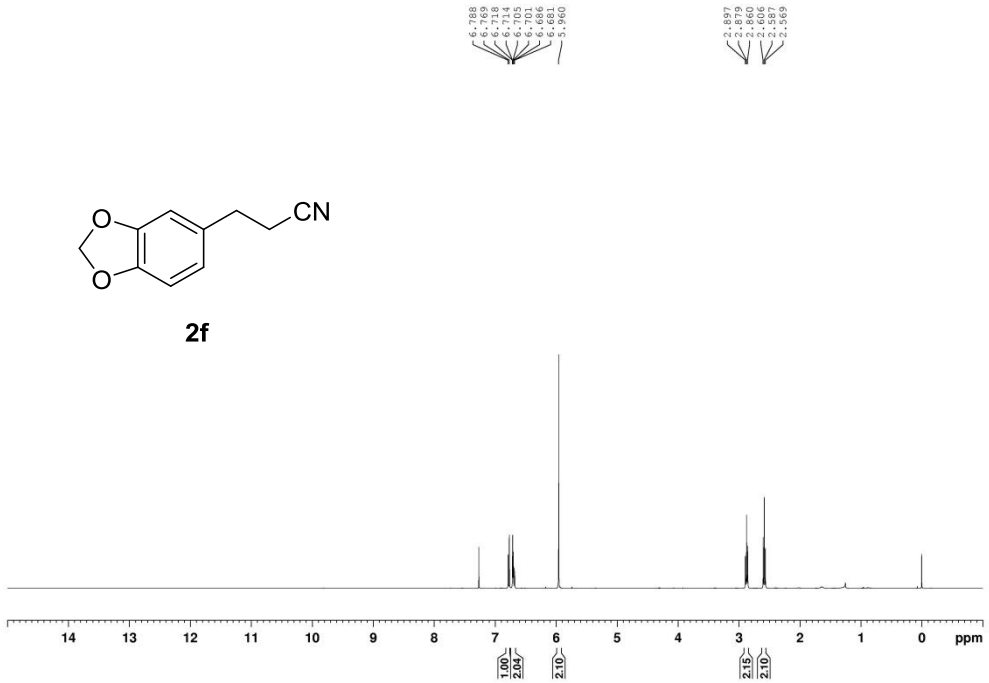

129.88
129.13
128.84
127.90
117.83
23.60
CN
2c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

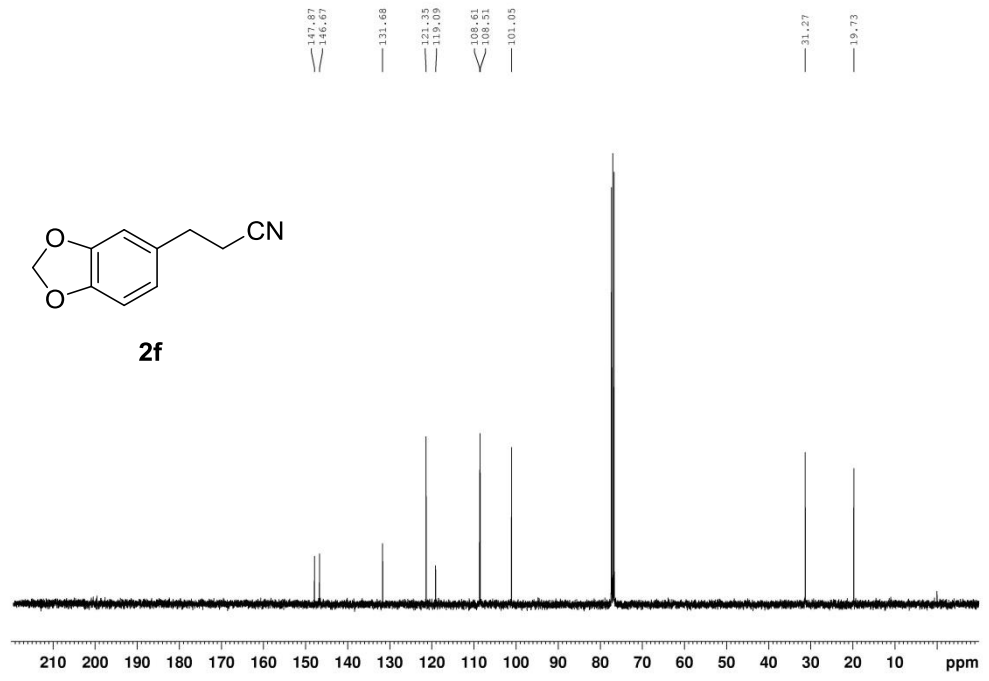

7.368
7.365
7.361
7.348
7.344
7.332
7.329
7.297
7.293
7.284
7.278
7.272
7.256
7.248
7.244
7.227
2.979
2.961
2.942
2.642
2.624
2.605
CN
2d
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.93
0.91
2.11
1.99
2.00

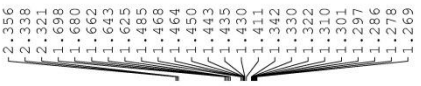

137.97
128.82
128.22
127.19
119.16
31.48
19.35
CN
2d
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

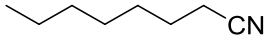

7.173
7.152
6.893
6.871
3.807
2.927
2.909
2.890
2.608
2.590
2.571
CN
O
2e
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.00
1.99
3.00
2.05
2.03


158.73
130.10
129.28
119.19
114.21
55.24
30.72
19.63
CN
O
2e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

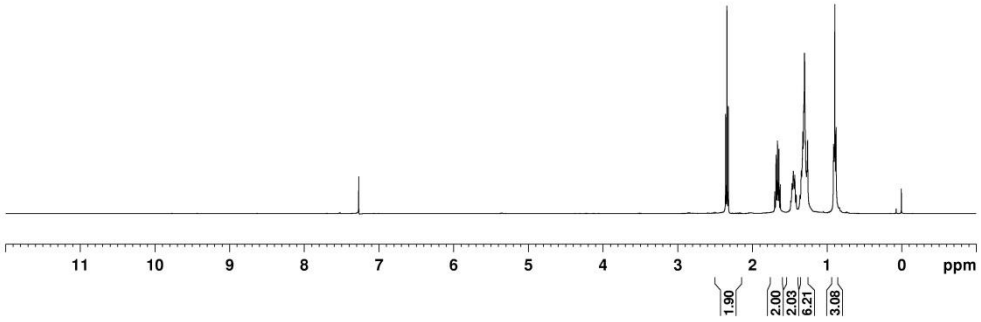

6.788
6.768
6.718
6.714
6.705
6.701
6.686
6.681
5.960
2.897
2.879
2.660
2.606
2.587
2.569
O
O
CN
2f
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
2.04
2.10
2.15
2.10


147.87
146.67
131.68
121.35
119.09
108.61
108.51
101.05
31.27
19.73
O
O
CN
2f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

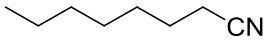

2.356
2.338
2.321
1.698
1.680
1.662
1.643
1.625
1.485
1.468
1.464
1.450
1.443
1.435
1.430
1.411
1.342
1.330
1.322
1.310
1.301
1.297
1.286
1.278
1.269


CN

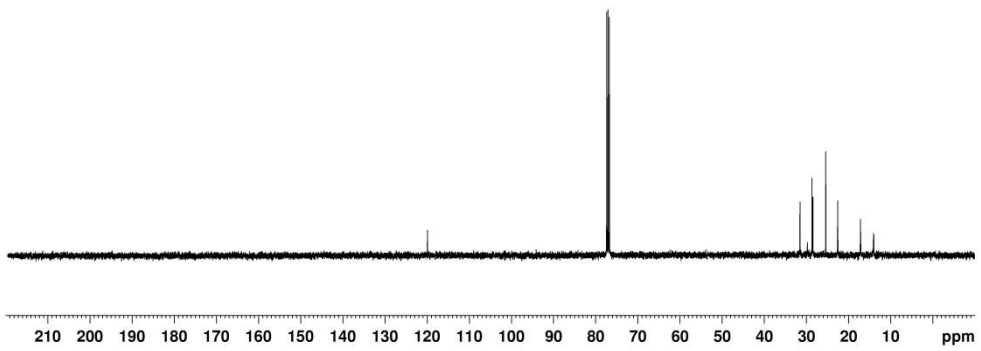
2g

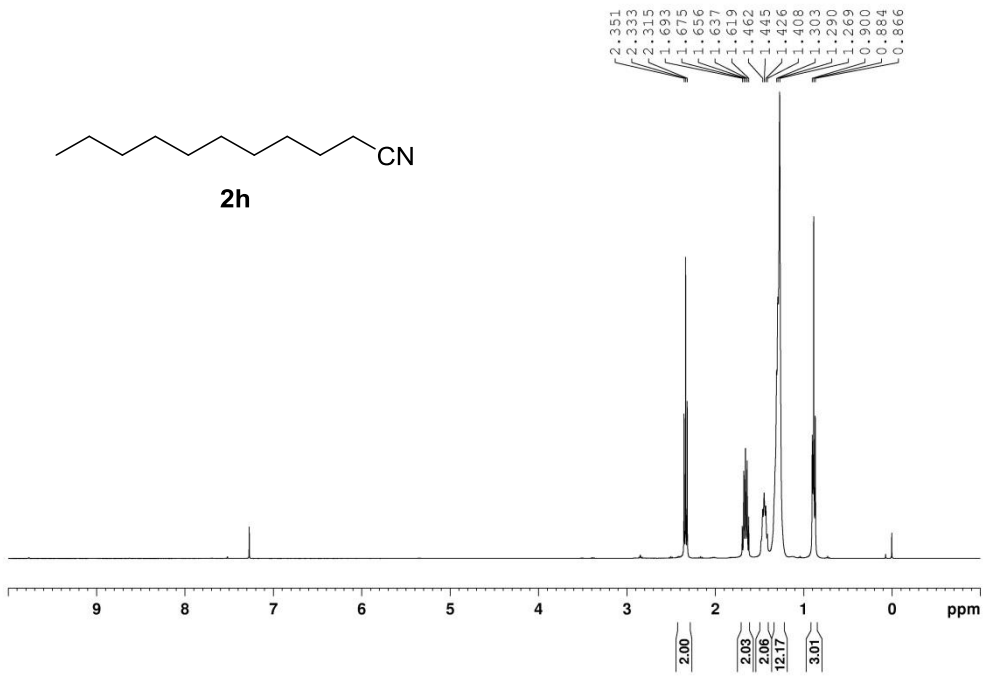

11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.90
2.00
2.03
6.21
3.08

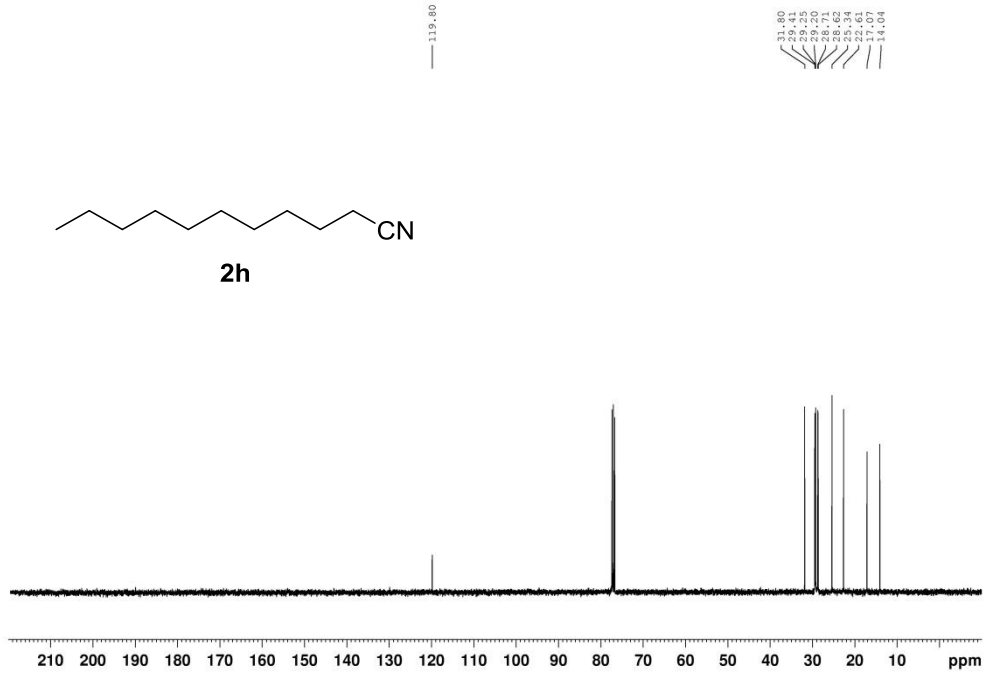

119.85
31.45
28.59
28.39
25.33
22.48
17.09
13.98

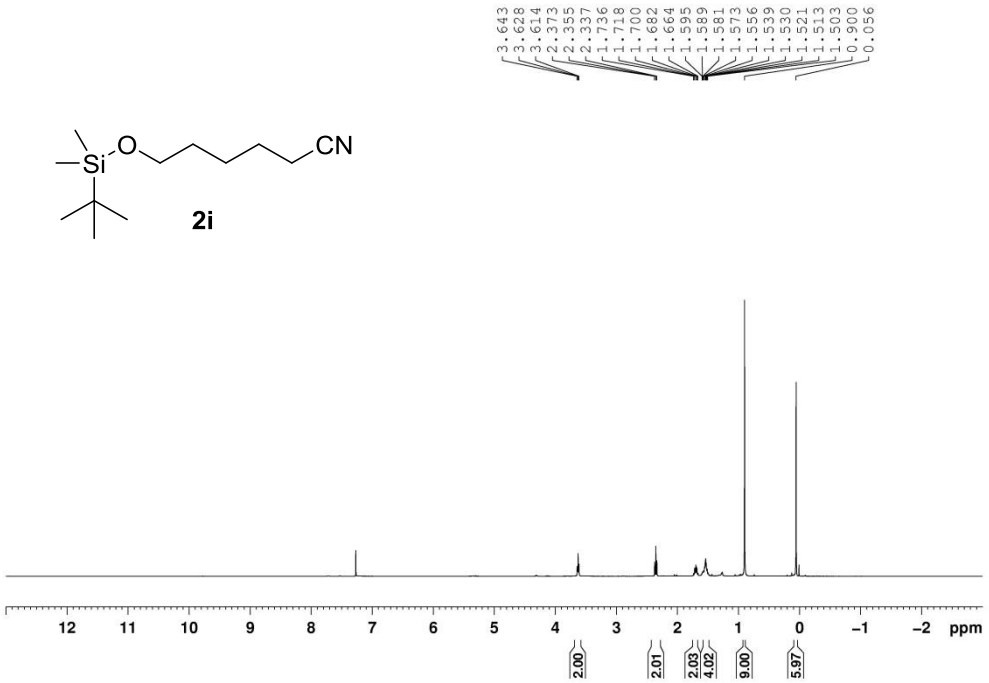

CN

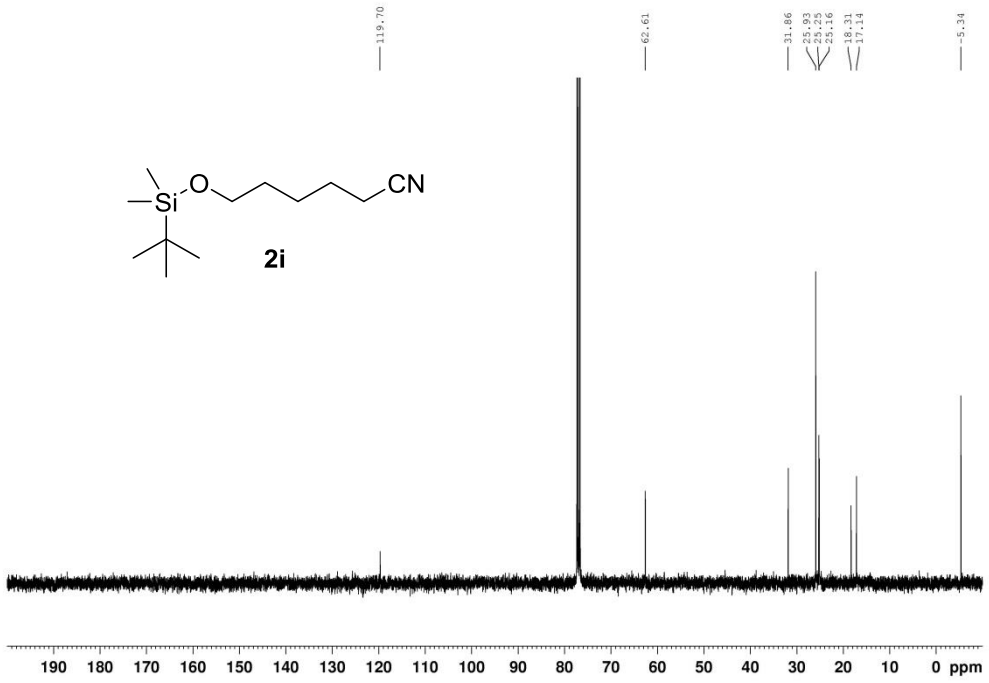
2g

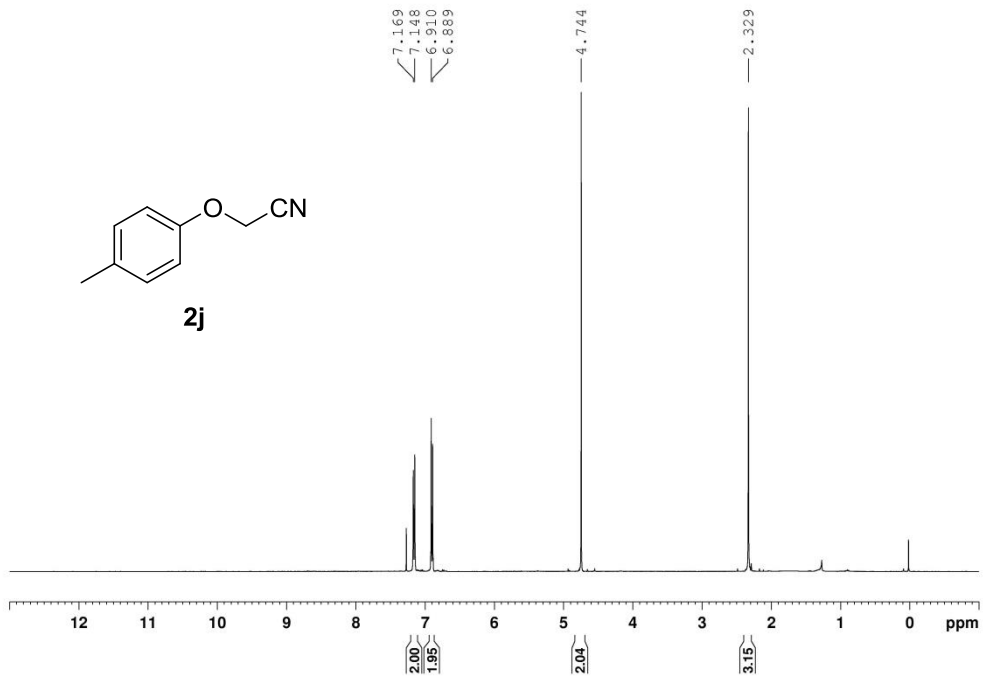

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


2.351
2.333
2.315
1.693
1.675
1.656
1.637
1.619
1.462
1.445
1.426
1.408
1.303
1.290
1.269
0.900
0.884
0.866
CN
2h
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.03
2.06
12.17
3.01

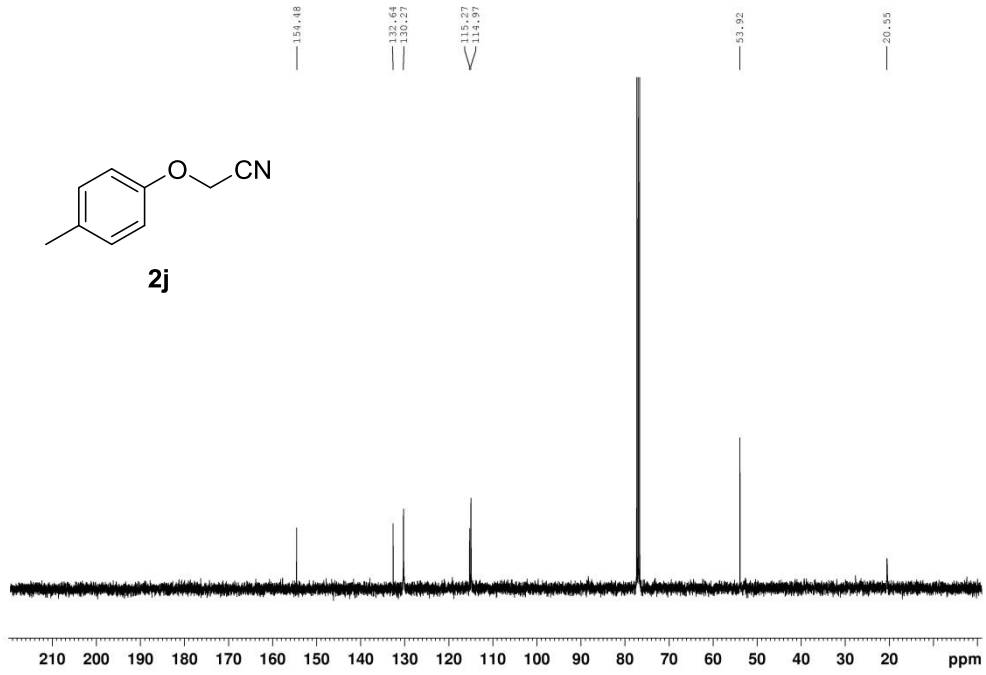

119.80
31.80
30.41
29.25
29.20
28.71
28.62
25.34
22.61
17.07
14.04
CN
2h
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


3.643
3.628
3.614
2.373
2.355
2.337
1.736
1.718
1.700
1.682
1.664
1.595
1.589
1.581
1.573
1.556
1.539
1.530
1.521
1.513
1.503
0.900
0.056
Si
O
CN
2i
12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 ppm
2.00
2.01
2.03
4.02
9.00
5.97


119.70
62.61
31.86
25.93
25.25
25.16
18.31
17.14
-5.34
Si
O
CN
2i
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

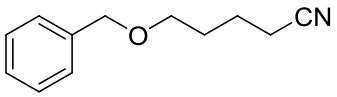

7.169
7.148
6.910
6.889
4.744
2.329
O
CN
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
1.95
2.04
3.15

2j

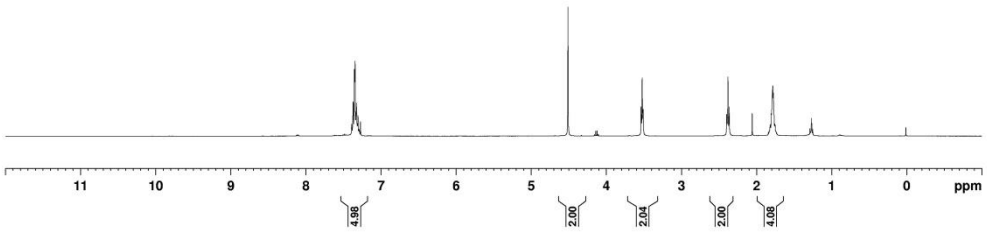

154.48
132.64
130.27
115.27
114.97
53.92
20.55
O
CN
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

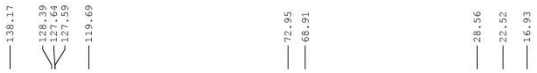
2j

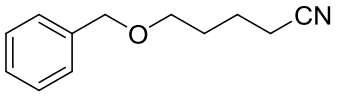

7.390
7.387
7.383
7.369
7.366
7.359
7.351
7.342
7.330
7.325
7.311
7.304
7.270
4.512
3.538
3.523
3.510
2.399
2.382
2.365
1.819
1.815
1.806
1.803
1.793
1.790
1.785
1.778
1.762
1.755


O
CN

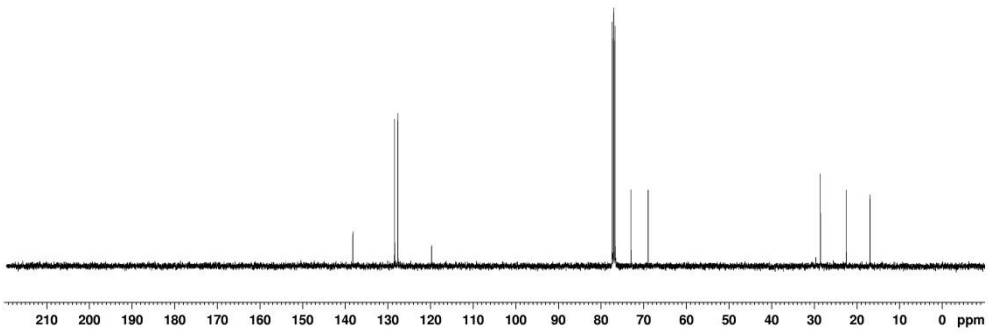
2k

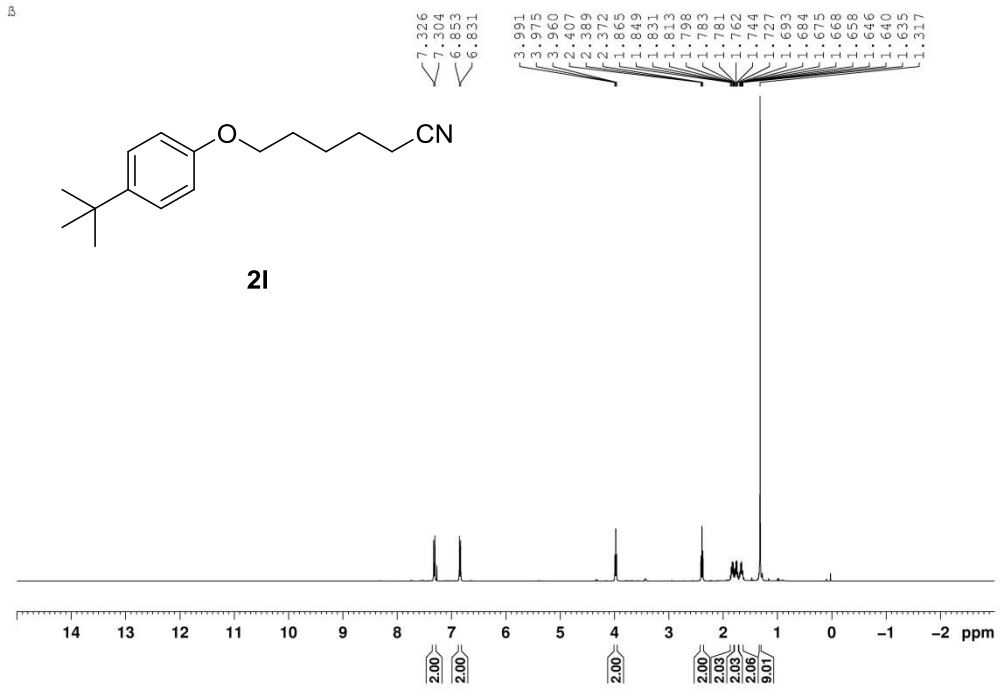

11
10
9
8
7
6
5
4
3
2
1
0
ppm
4.98
2.00
2.04
2.00
4.08


138.17
128.39
127.64
127.59
119.69
72.95
68.91
28.56
22.52
16.93

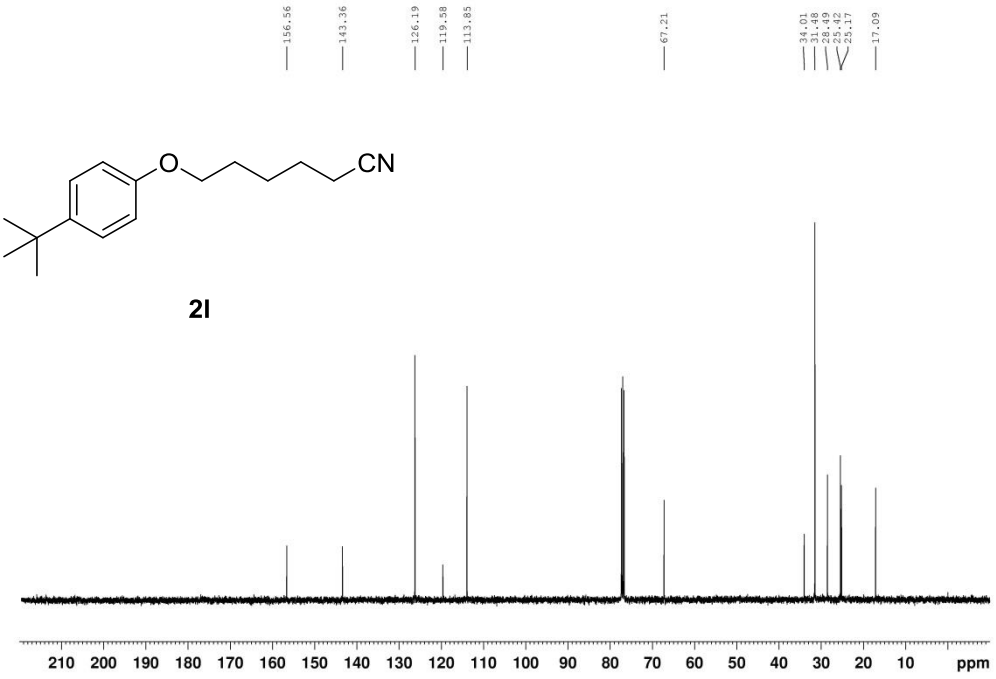

O
CN

2k

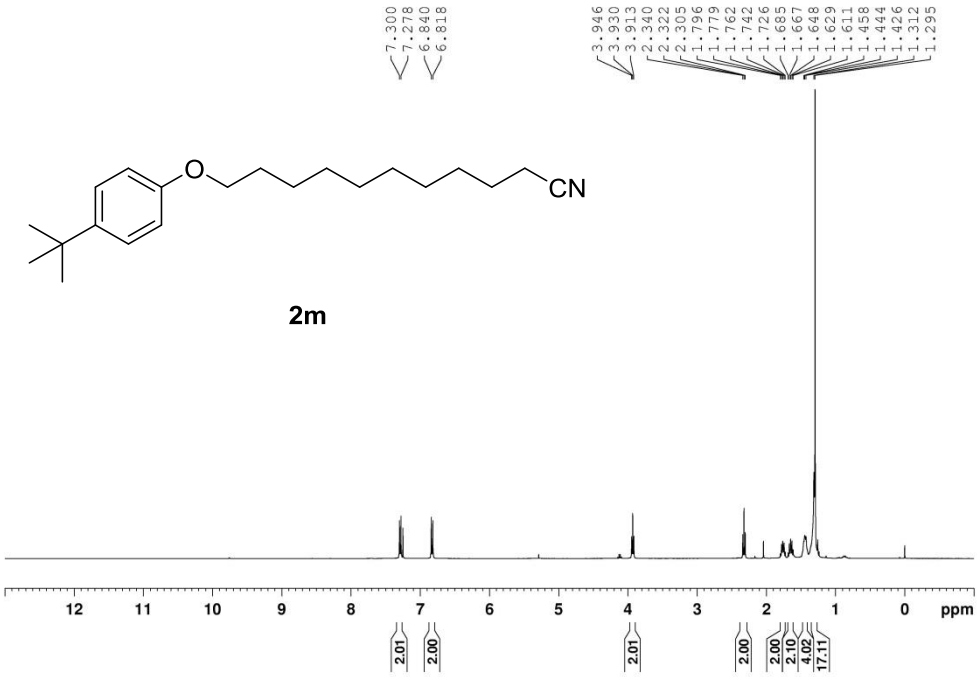

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


7.326
7.304
6.853
6.831
3.991
3.975
3.960
2.407
2.389
2.372
1.865
1.849
1.831
1.813
1.798
1.783
1.781
1.762
1.744
1.727
1.693
1.684
1.675
1.668
1.658
1.646
1.640
1.635
1.317
O
CN
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 ppm
2.00
2.00
2.00
2.00
2.05
2.03
2.06
9.01

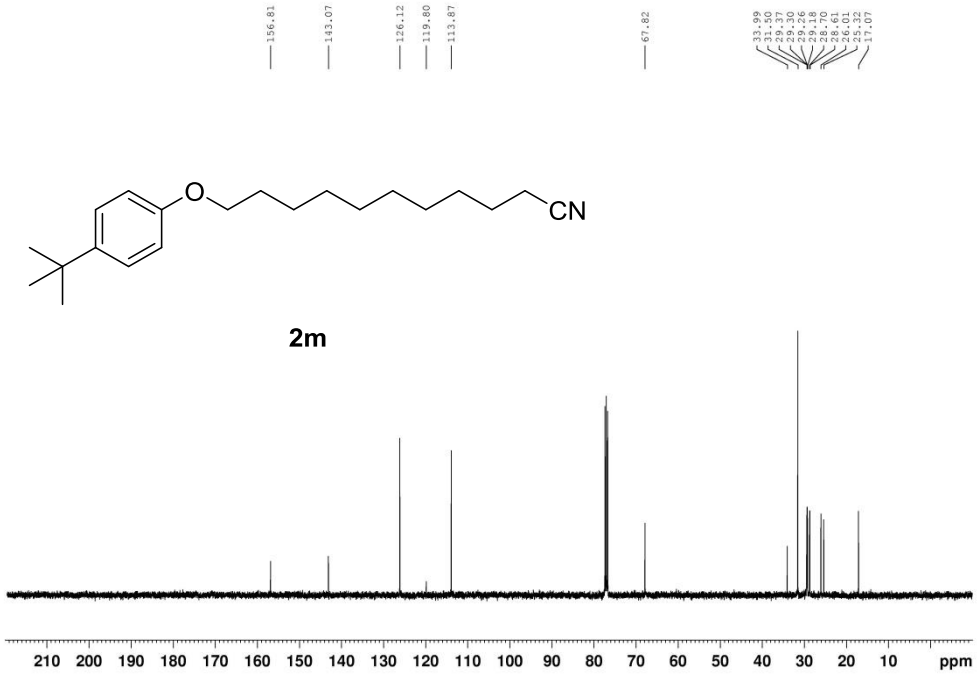
2l


156.56
143.36
126.19
119.58
113.85
67.21
34.01
31.48
28.49
25.42
25.17
17.09
O
CN
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

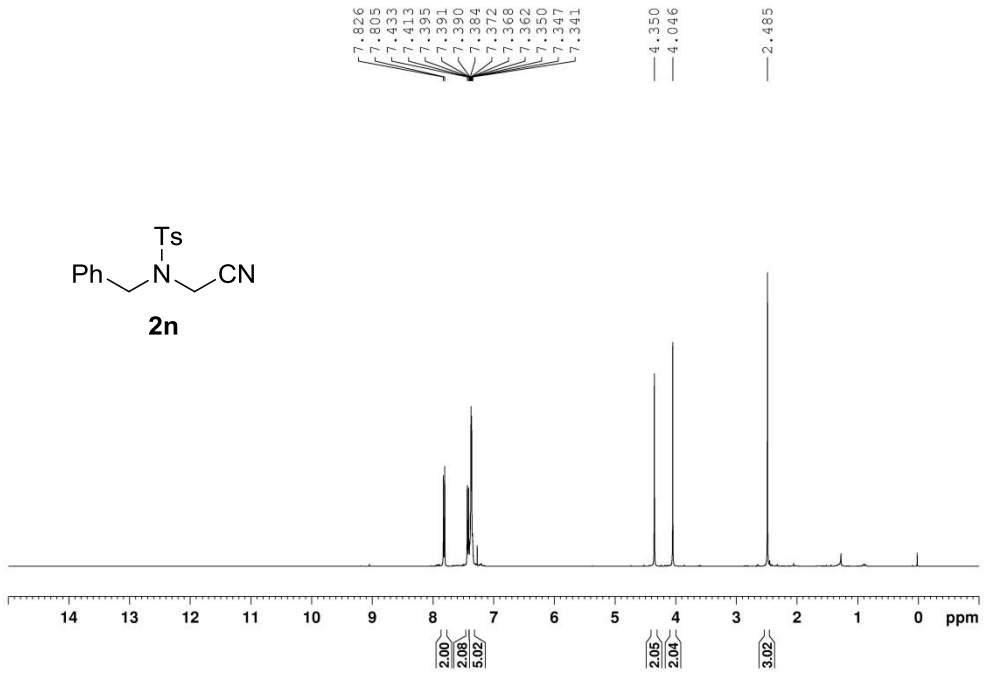
2l

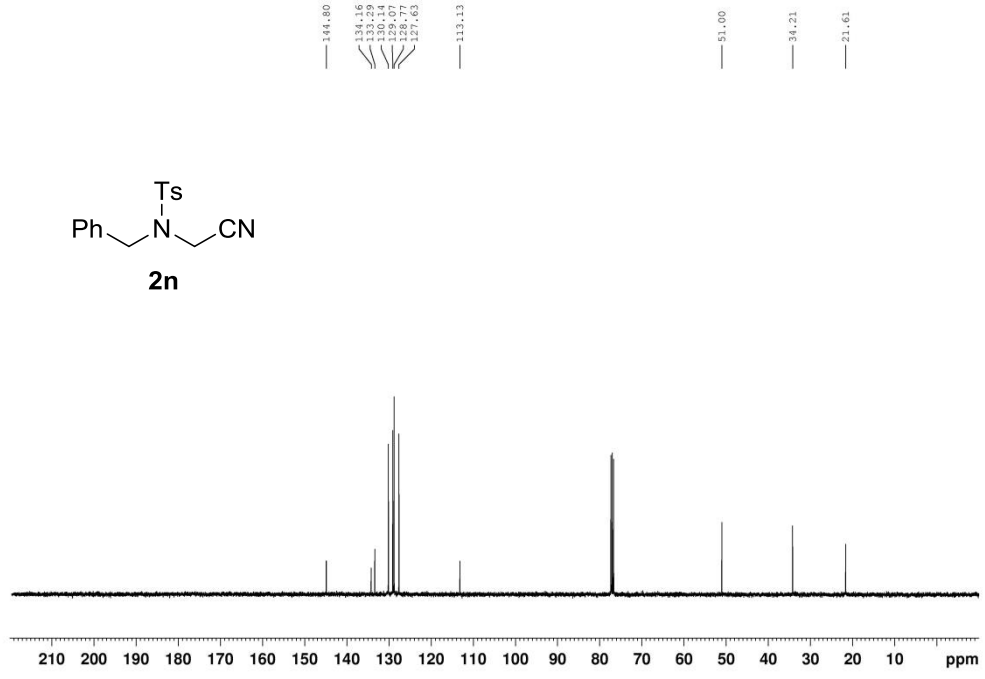

7.300
7.278
6.840
6.818
3.946
3.930
3.913
2.340
2.322
2.305
1.796
1.779
1.762
1.742
1.726
1.685
1.667
1.648
1.629
1.611
1.458
1.444
1.426
1.312
1.295
O
CN
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.01
2.00
2.01
2.00
2.00
2.10
4.02
17.11

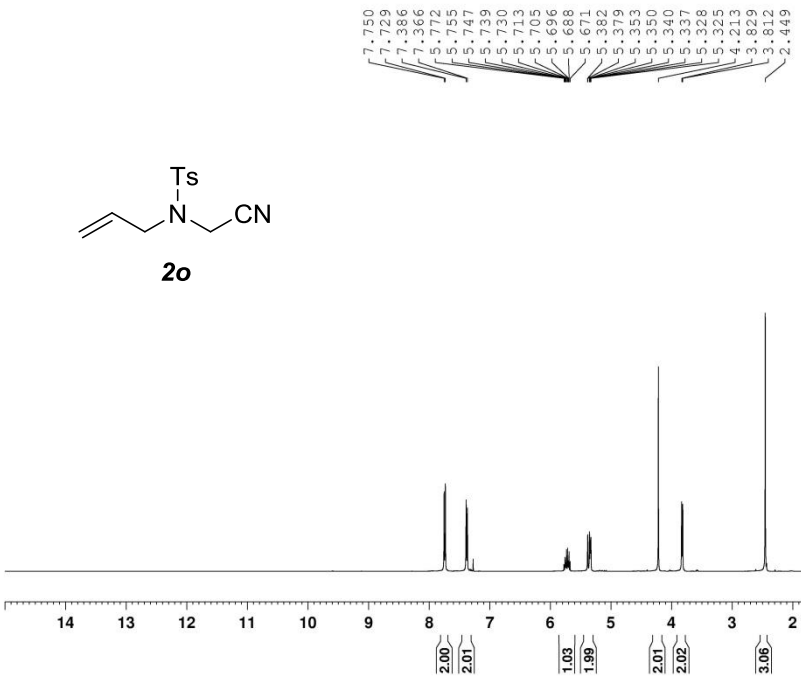
2m

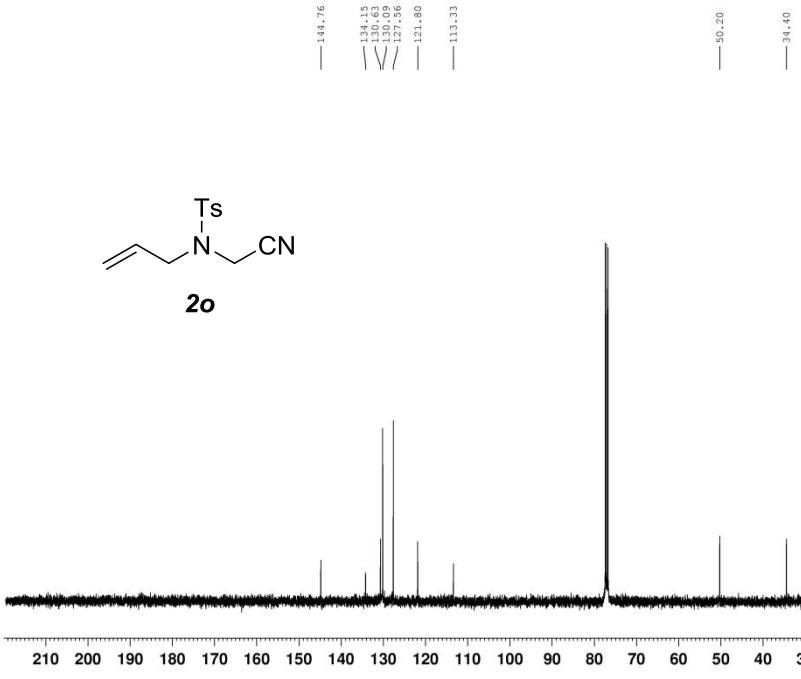

156.81
143.07
126.12
119.80
113.87
67.82
33.99
31.50
29.37
29.30
29.26
29.18
28.70
28.61
26.01
25.32
21.07
O
CN
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

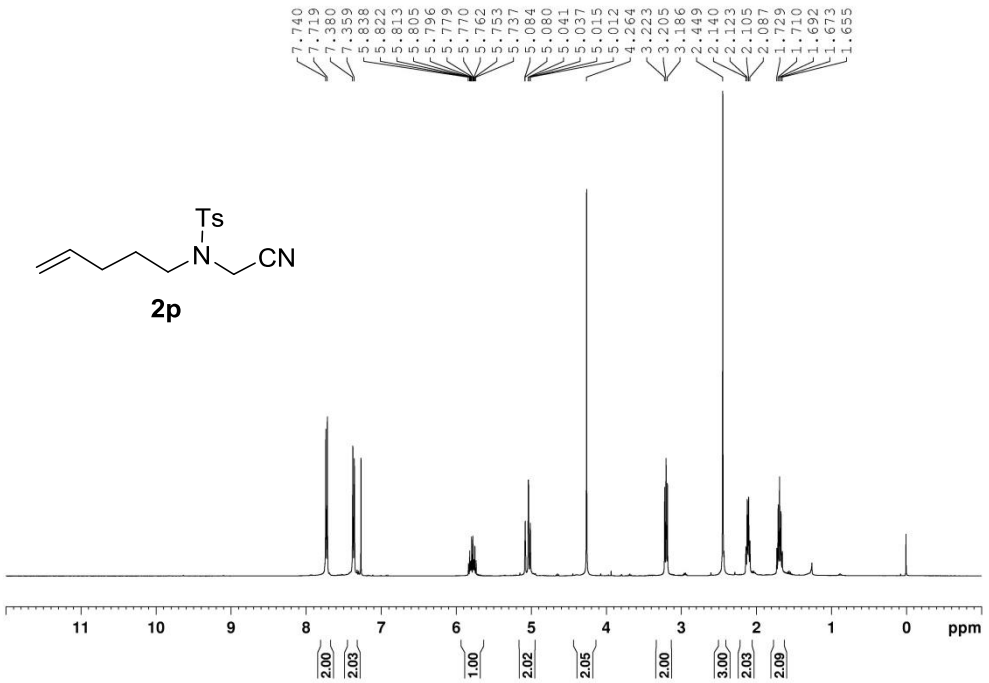
2m

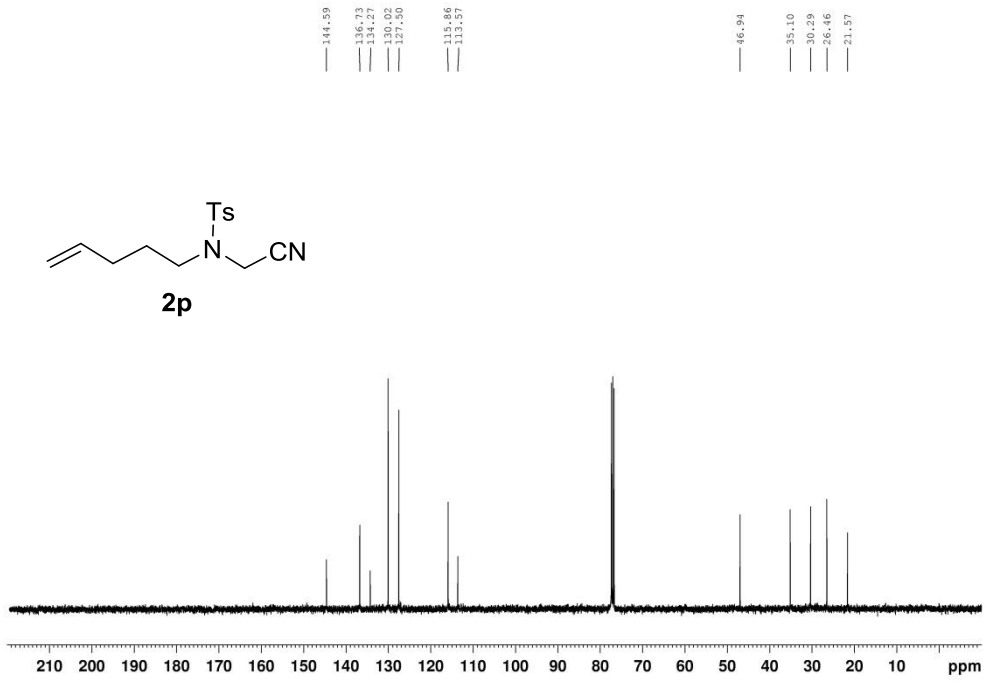

7.826
7.805
7.433
7.413
7.395
7.391
7.390
7.384
7.372
7.368
7.362
7.350
7.347
7.341
4.350
4.046
2.485
Ts
Ph
N
CN
2n
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.00
2.08
5.02
2.05
2.04
3.02

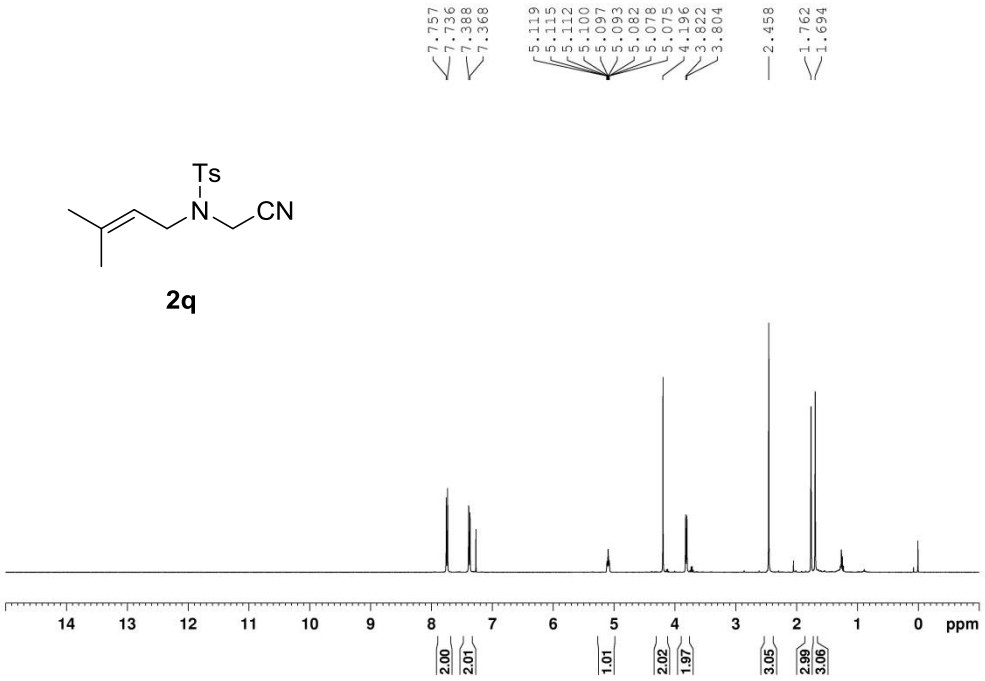

144.80
134.16
133.29
130.14
129.07
128.77
127.63
113.13
51.00
34.21
21.61
Ts
Ph
N
CN
2n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.750
7.729
7.386
7.366
5.772
5.755
5.747
5.739
5.730
5.713
5.705
5.696
5.688
5.671
5.382
5.379
5.353
5.350
5.340
5.337
5.328
5.325
4.213
3.829
3.812
2.449
Ts
N
CN
2o
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.00
2.01
1.03
1.99
2.01
2.02
3.06

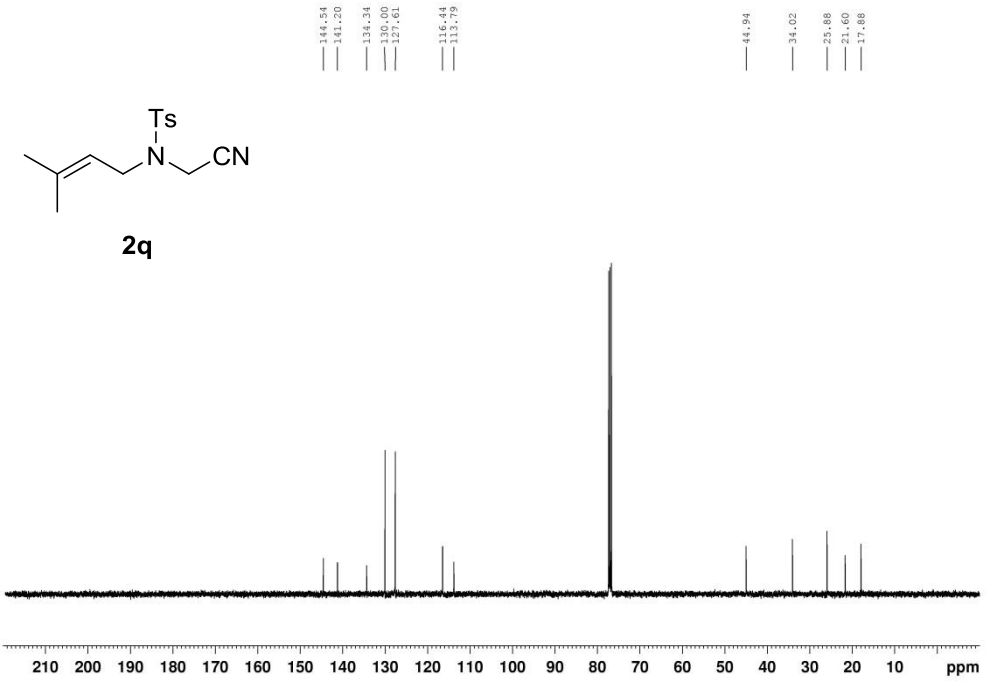

144.76
134.15
130.63
130.09
127.56
121.80
113.33
50.20
34.40
21.61
Ts
N
CN
2o
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.740
7.719
7.380
7.359
5.838
5.822
5.813
5.805
5.796
5.779
5.770
5.762
5.753
5.737
5.084
5.080
5.041
5.037
5.015
5.012
4.264
3.223
3.205
3.186
2.449
2.140
2.123
2.105
2.087
1.729
1.710
1.692
1.673
1.655
Ts
N
CN
2p
11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.00 2.03 1.00 2.02 2.05 2.00 3.00 2.03 2.09

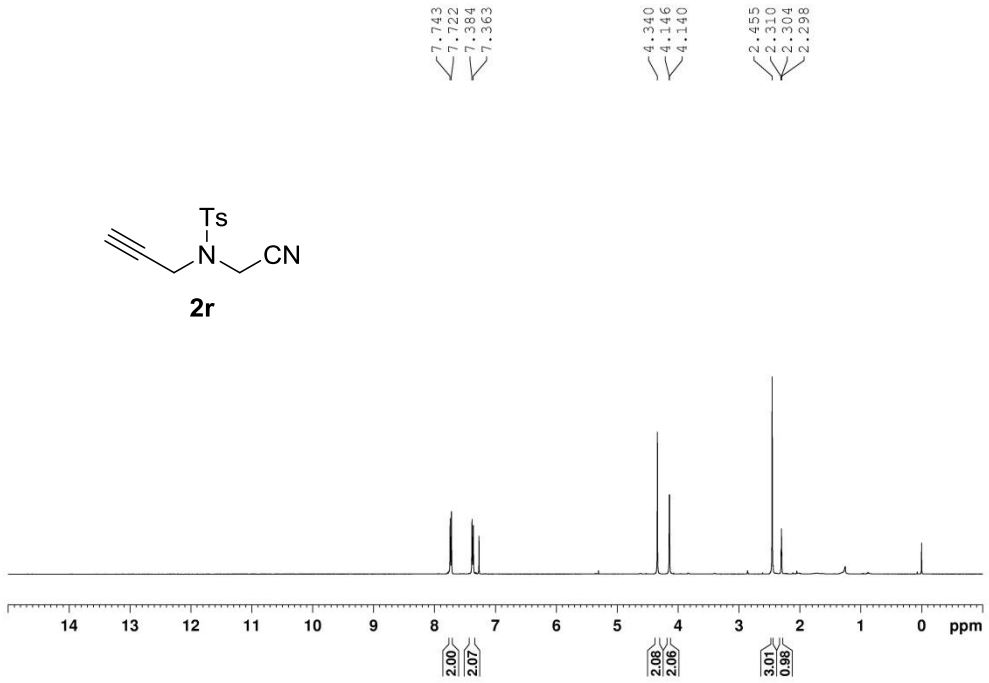

144.59
136.23
134.27
130.02
127.50
115.86
113.57
46.94
35.10
30.29
26.46
21.57
Ts
N
CN
2p
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

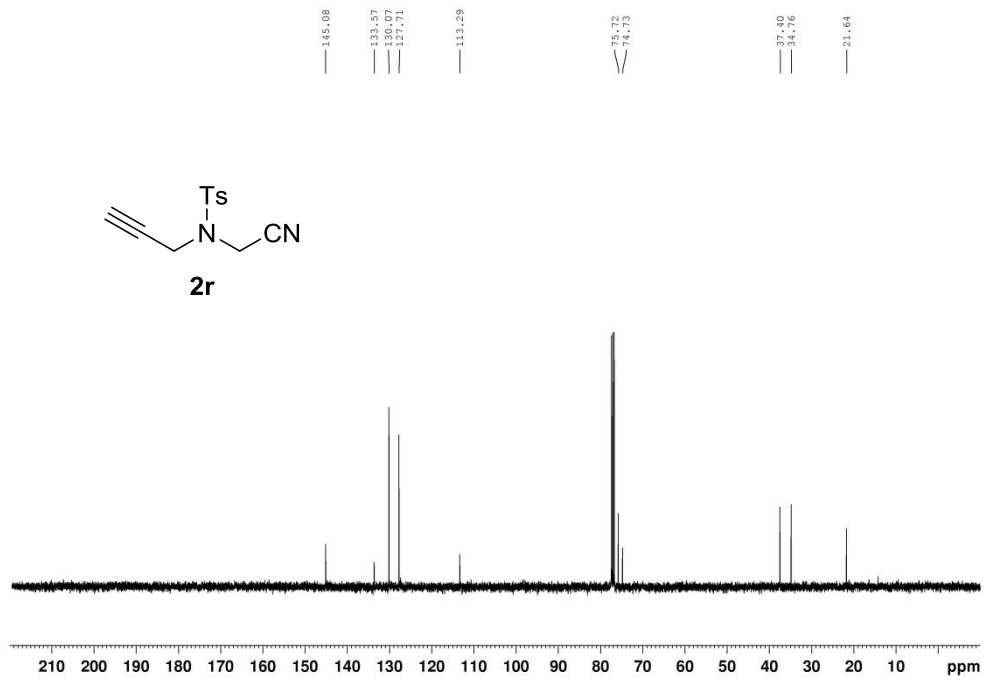

7.757
7.736
7.388
7.368
5.119
5.115
5.112
5.100
5.097
5.093
5.082
5.078
5.075
4.196
3.822
3.804
2.458
1.762
1.694
Ts
N
CN
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.00
2.01
1.01
2.02
1.97
3.05
2.99
3.06

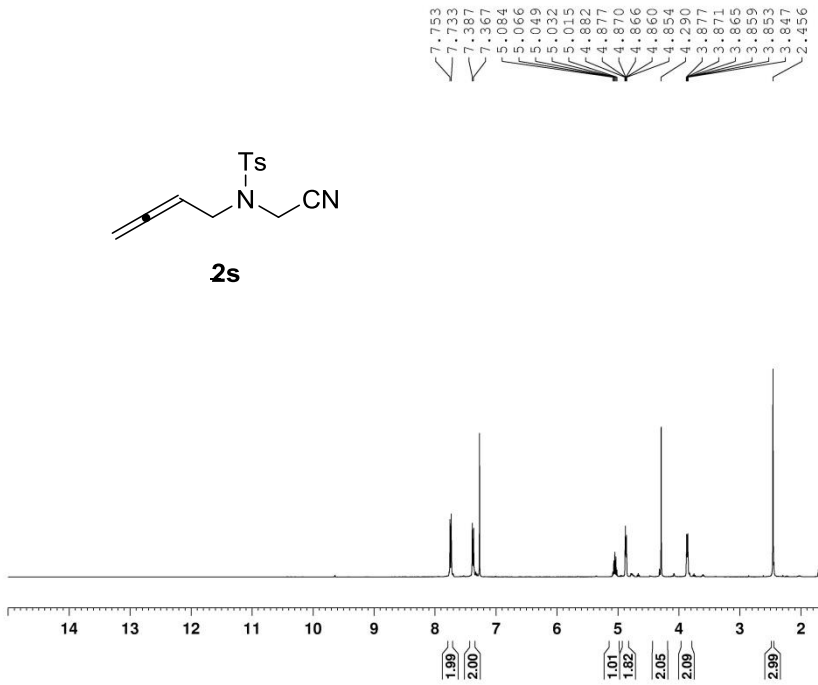
2q

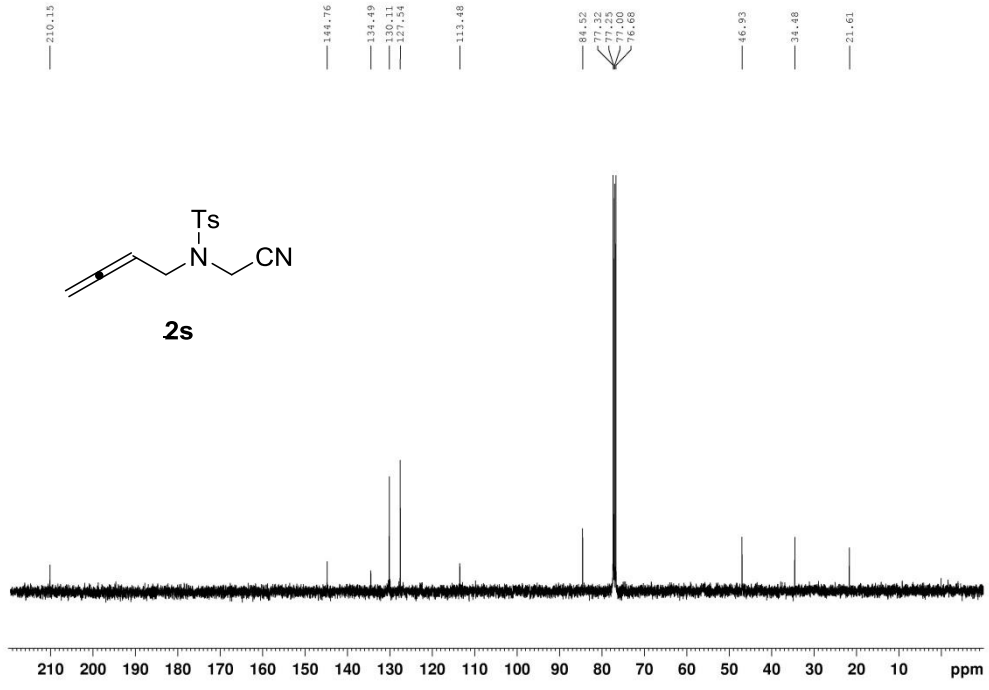

144.54
141.20
134.34
130.00
127.61
116.44
113.79
44.94
34.02
25.88
21.60
17.88
Ts
N
CN
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

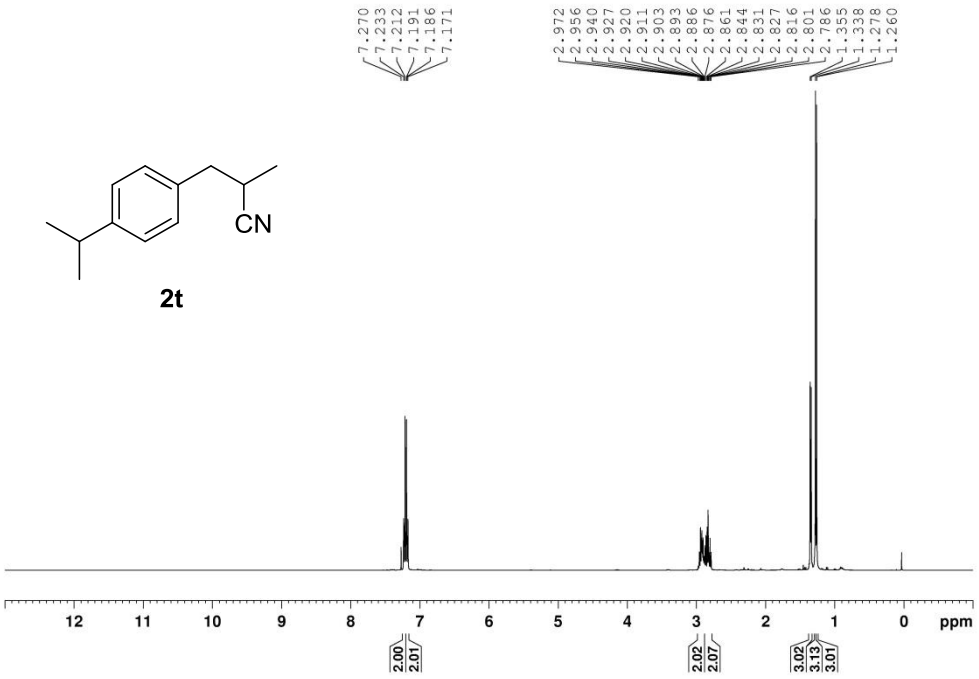
2q


7.743
7.722
7.384
7.363
4.340
4.146
4.140
2.455
2.310
2.304
2.298
Ts
N
CN
2r
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.00
2.07
2.08
2.06
3.01
0.98

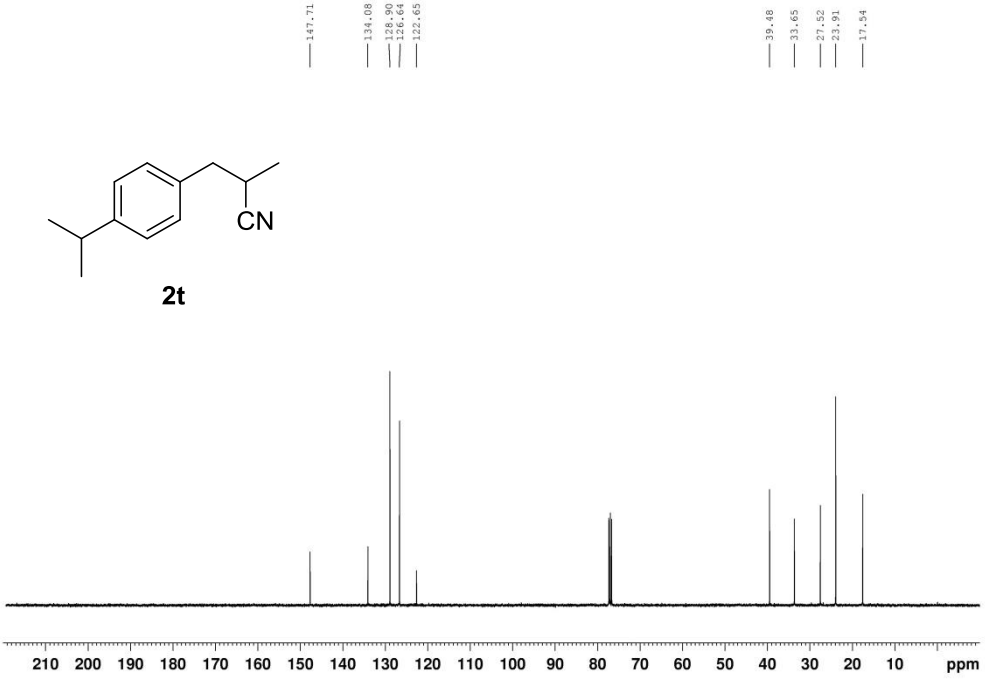

145.08
133.57
130.07
127.71
113.29
75.72
74.73
37.40
34.76
21.64
Ts
N
CN
2r
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.753
7.733
7.387
7.367
5.084
5.066
5.049
5.032
5.015
4.882
4.877
4.870
4.866
4.860
4.854
4.290
3.877
3.871
3.865
3.859
3.853
3.847
2.456
Ts
N
CN
2s
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.99
2.00
1.01
1.82
2.05
2.09
2.99

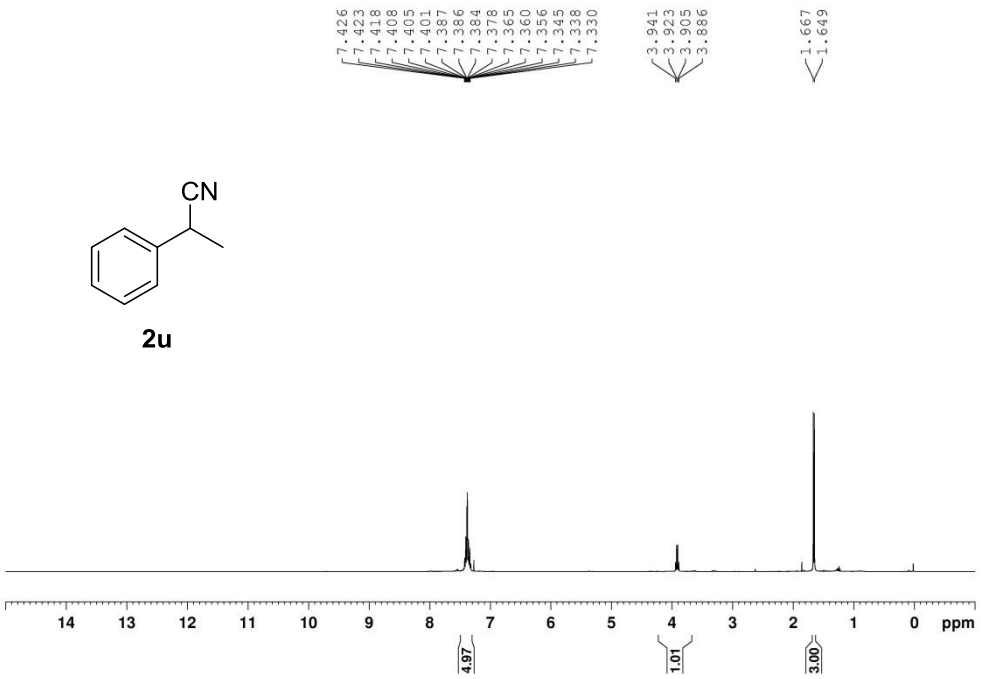

210.15
144.76
134.49
130.11
127.54
113.48
84.52
77.32
77.25
77.00
76.68
46.93
34.48
21.61
Ts
N
CN
2s
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

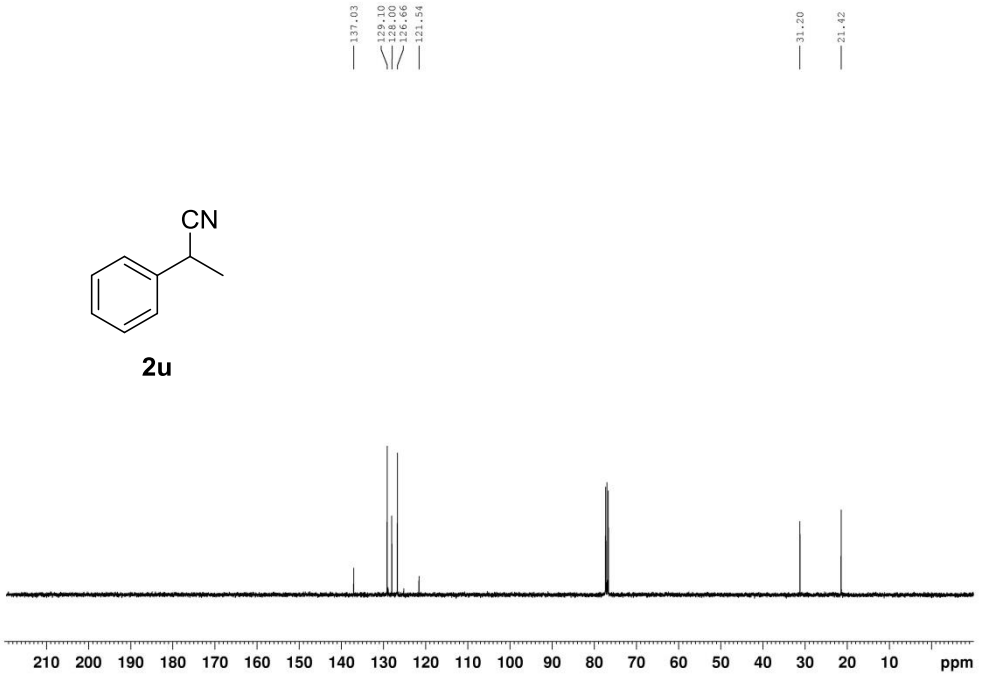

7.270
7.233
7.212
7.191
7.186
7.171
2.972
2.956
2.940
2.927
2.920
2.911
2.903
2.893
2.886
2.876
2.861
2.844
2.831
2.827
2.816
2.801
2.786
1.355
1.338
1.278
1.260
CN
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.00
2.01
2.02
2.07
3.02
3.13
3.01

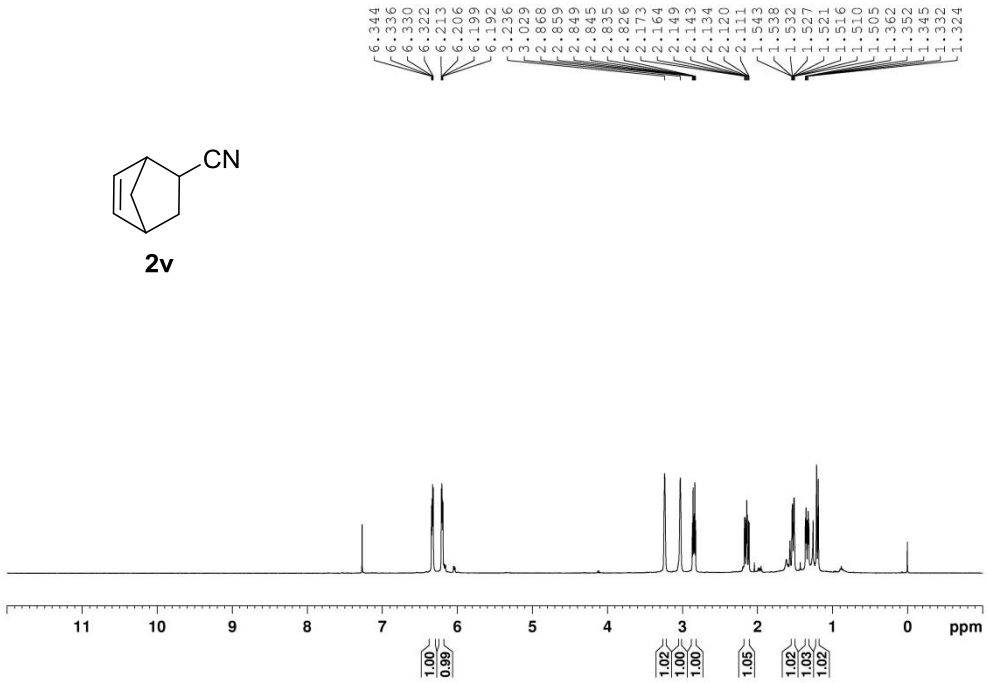
2t

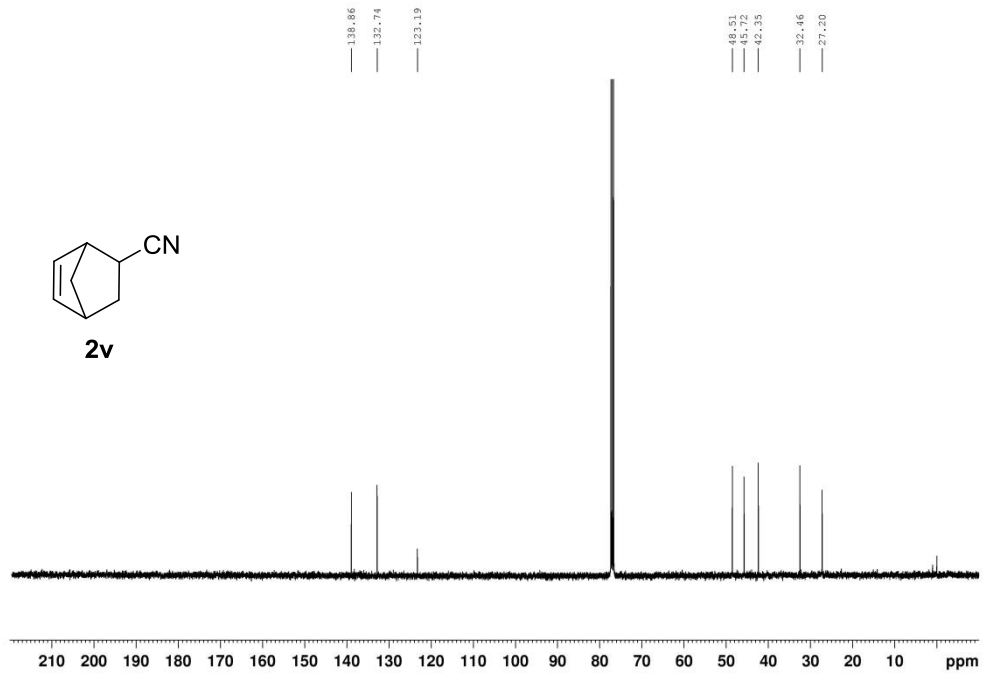

147.71
134.08
128.90
126.64
122.65
39.48
33.65
27.52
23.91
17.54
CN
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

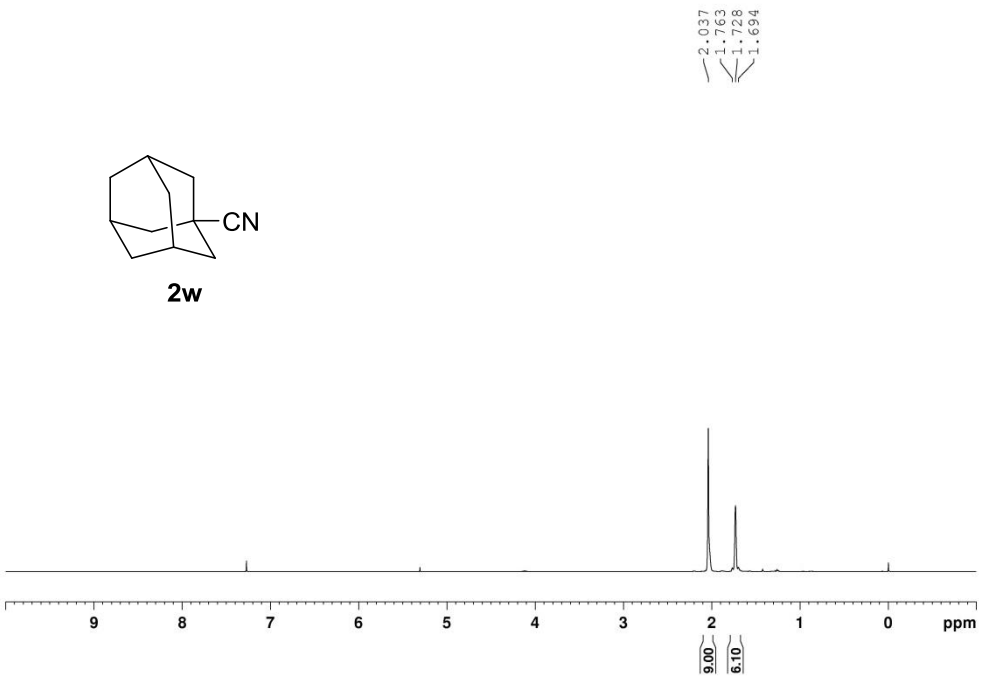
2t

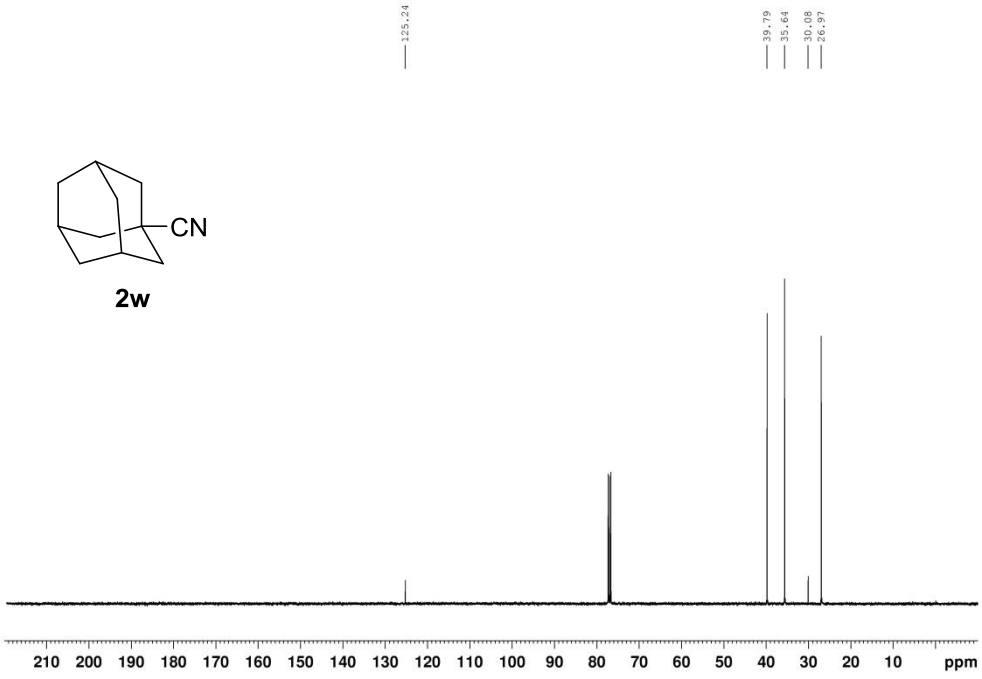

7.426
7.423
7.418
7.408
7.405
7.401
7.387
7.386
7.384
7.378
7.365
7.360
7.356
7.345
7.338
7.330
3.941
3.923
3.905
3.886
1.667
1.649
CN
2u
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
4.97
1.01
3.00


137.03
129.10
128.00
126.66
121.54
31.20
21.42
CN
2u
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

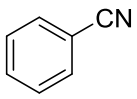

6.344
6.336
6.330
6.322
6.213
6.206
6.199
6.192
3.236
3.029
2.868
2.859
2.849
2.845
2.835
2.826
2.173
2.164
2.149
2.143
2.134
2.120
2.111
1.543
1.538
1.532
1.527
1.521
1.516
1.510
1.505
1.362
1.352
1.345
1.332
1.324
CN
2v
11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
0.99
1.02
1.00
1.00
1.05
1.02
1.03
1.02


138.86
132.74
123.19
48.51
45.72
42.35
32.46
27.20
CN
2v
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

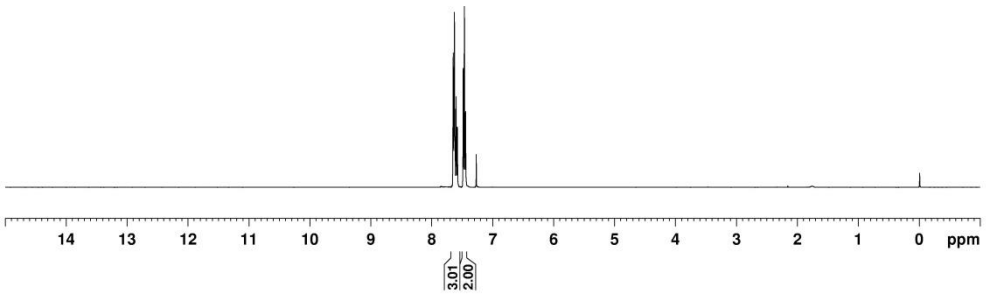

2.037
1.763
1.728
1.694
CN
2w
9
8
7
6
5
4
3
2
1
0
ppm
9.00
6.10


125.24
39.79
35.64
30.08
26.97
CN
2w
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

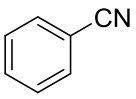

7.648
7.647
7.629
7.626
7.618
7.599
7.582
7.580
7.484
7.465
7.445


CN

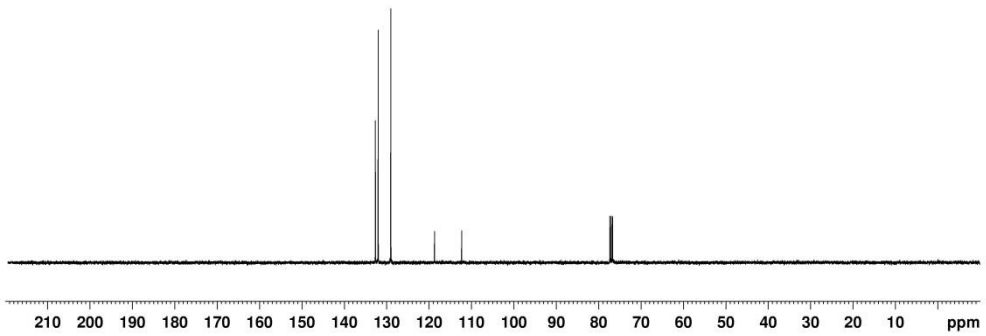
4a

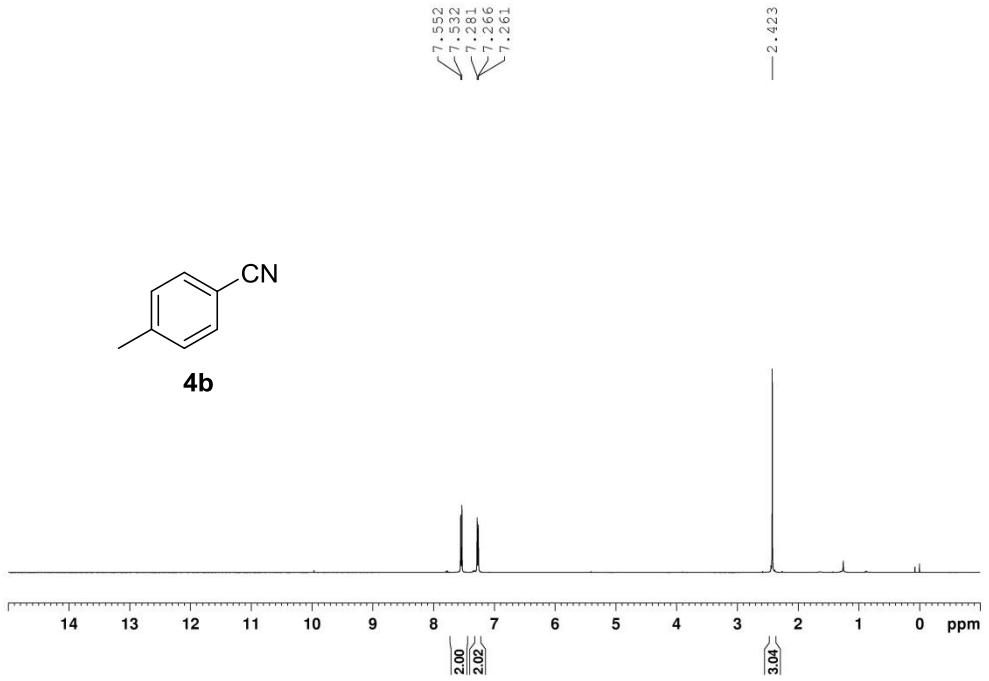

14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
3.01
2.00

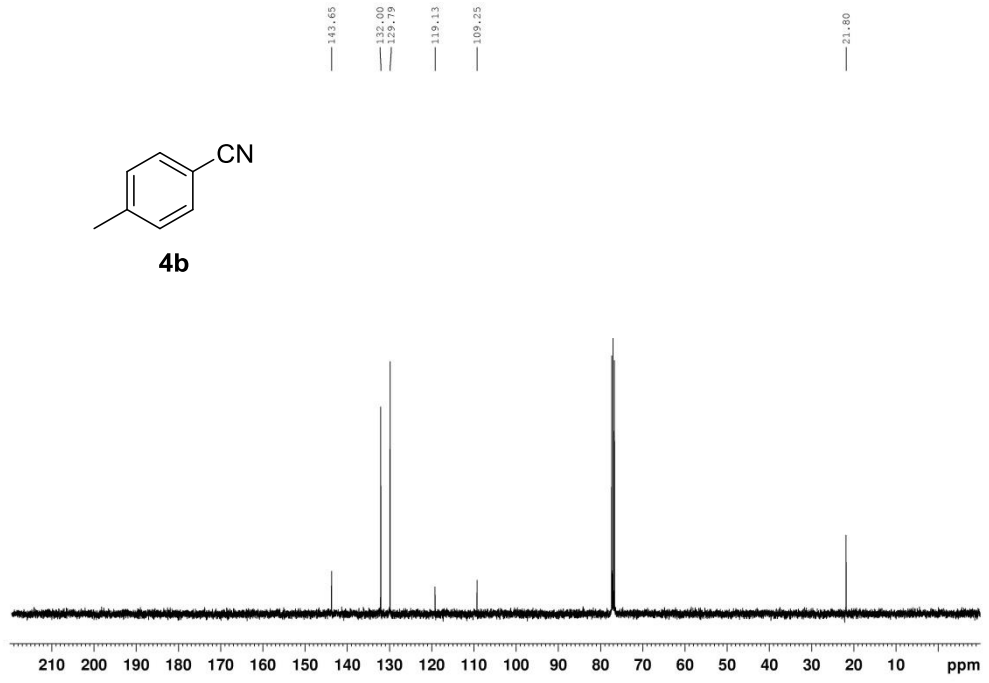

132.65
131.88
128.99
118.69
112.28

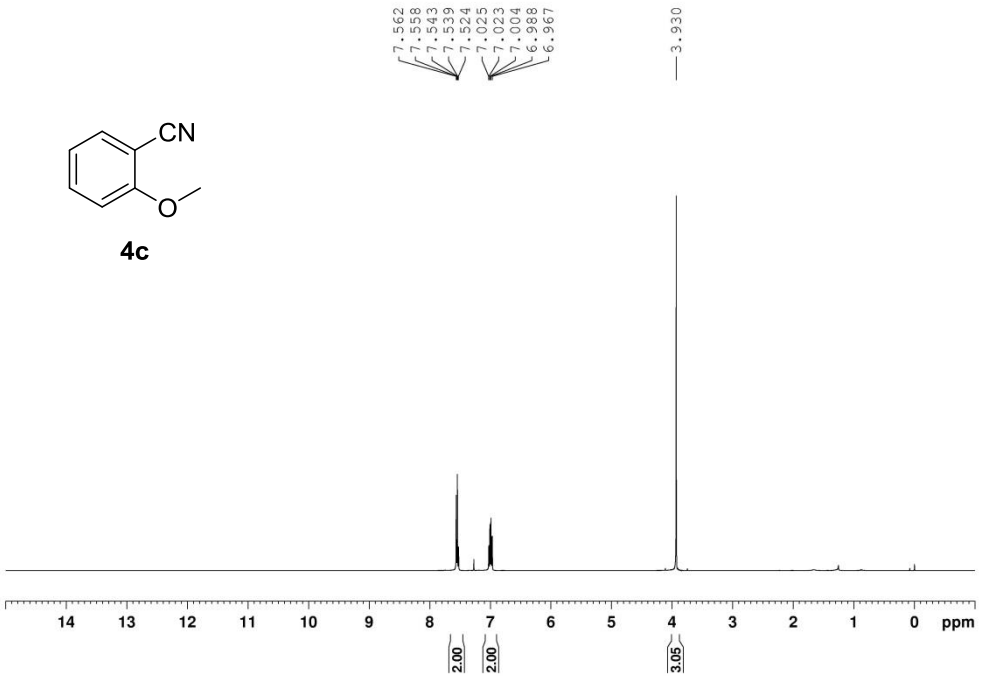

CN

4a

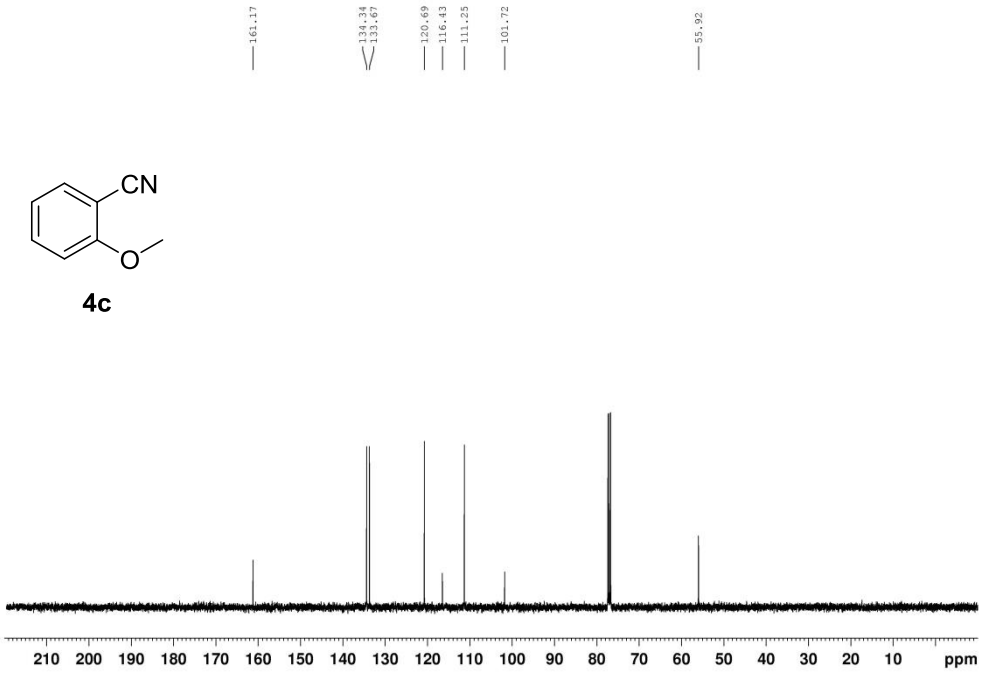

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.552
7.532
7.281
7.266
7.261
2.423
CN
4b
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.00
2.02
3.04

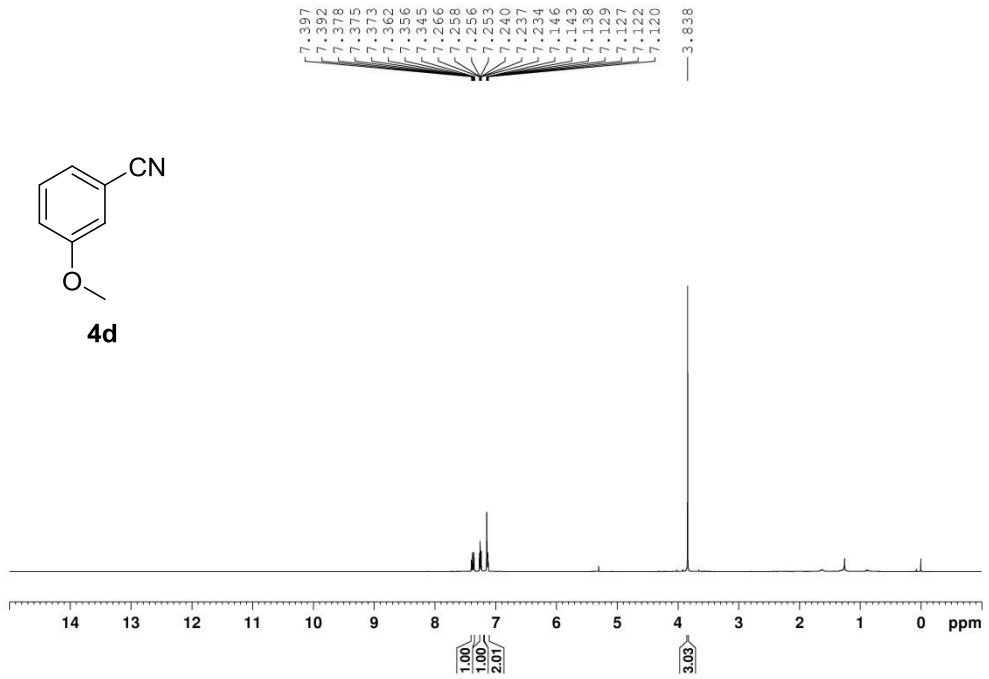

143.65
132.00
129.79
119.13
109.25
21.80
CN
4b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

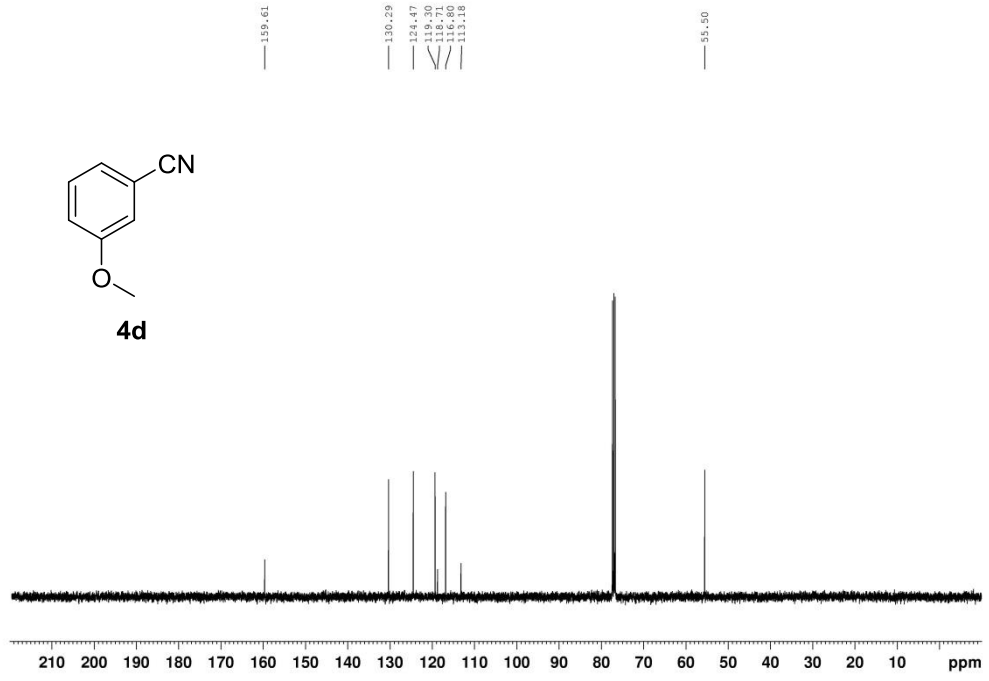

7.562
7.558
7.543
7.539
7.524
7.025
7.023
7.004
6.988
6.967
3.930
CN
O
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.00
2.00
3.05

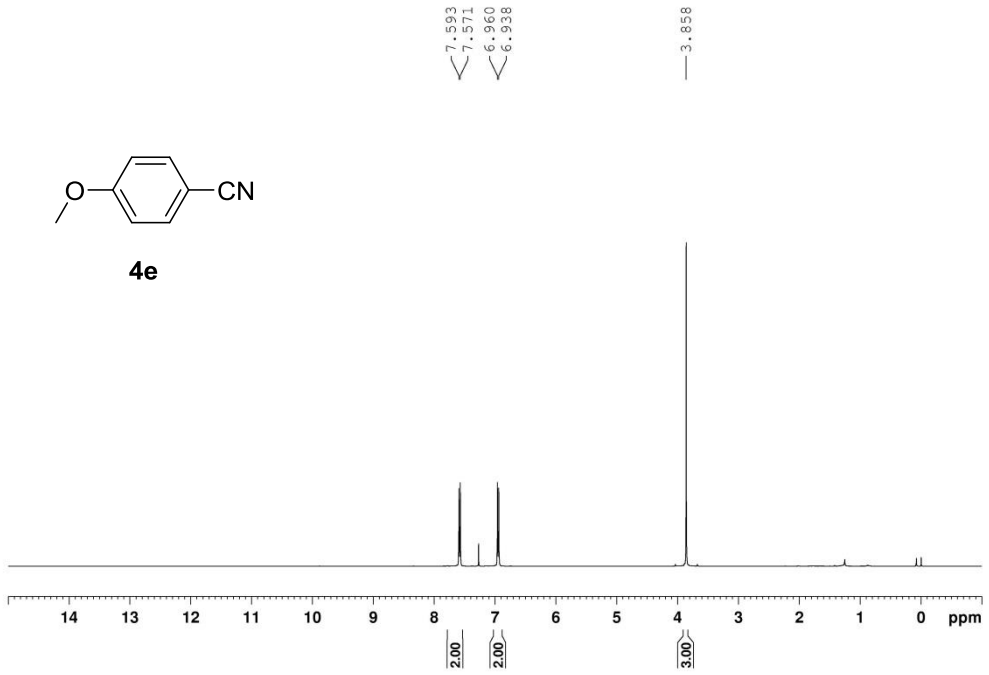
4c


161.17
134.34
133.67
120.69
116.43
111.25
101.72
55.92
CN
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

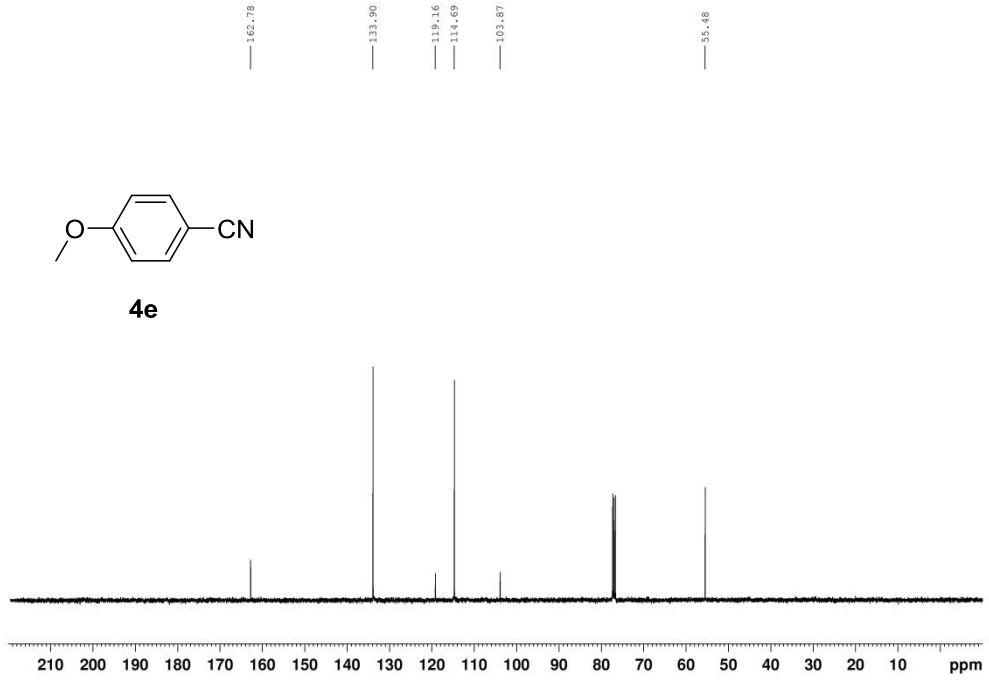
4c


7.397
7.392
7.378
7.375
7.373
7.362
7.356
7.345
7.266
7.258
7.256
7.253
7.240
7.237
7.234
7.146
7.143
7.138
7.129
7.127
7.122
7.120
3.838
CN
O
4d
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
1.00
2.01
3.03


159.61
130.29
124.47
119.30
118.71
116.80
113.18
55.50
CN
O
4d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

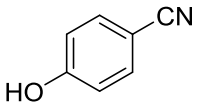

7.593
7.571
6.960
6.938
3.858
O
CN
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.00
2.00
3.00

4e

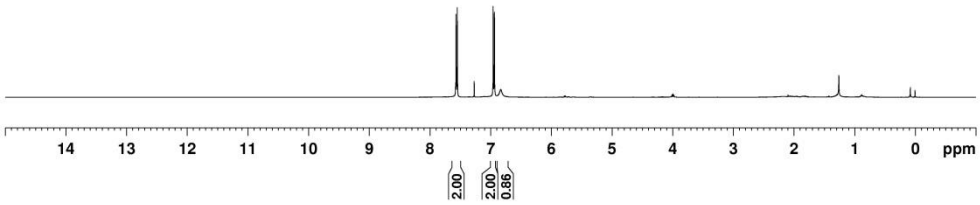

162.78
133.90
119.16
114.69
103.87
55.48
O
CN
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

4e

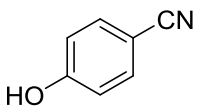

7.577
7.570
7.565
7.553
7.548
7.542
6.964
6.957
6.952
6.940
6.935
6.929
6.832


CN
HO

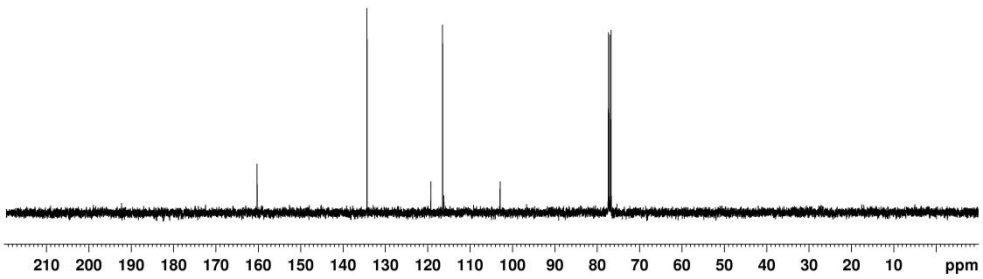
4f

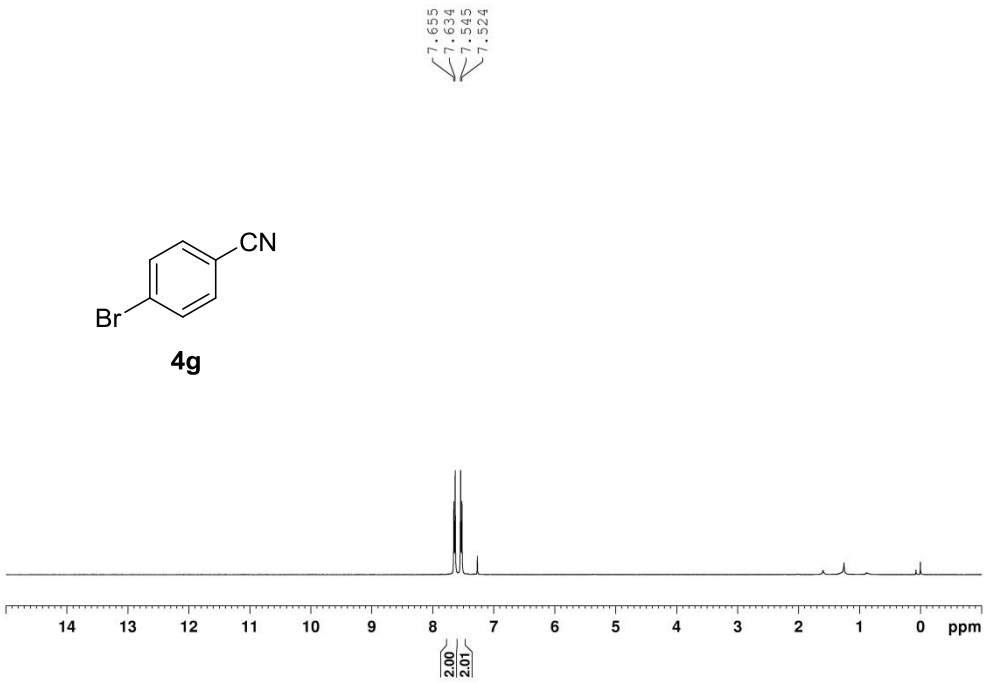

14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.00
2.00
0.86

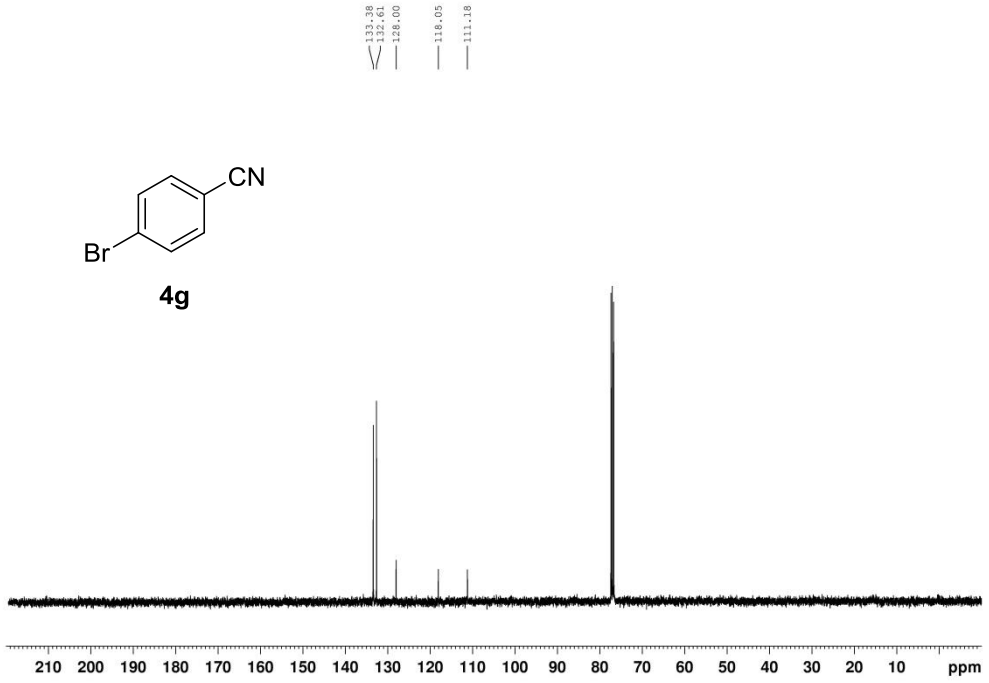

160.28
134.31
119.24
116.46
102.89

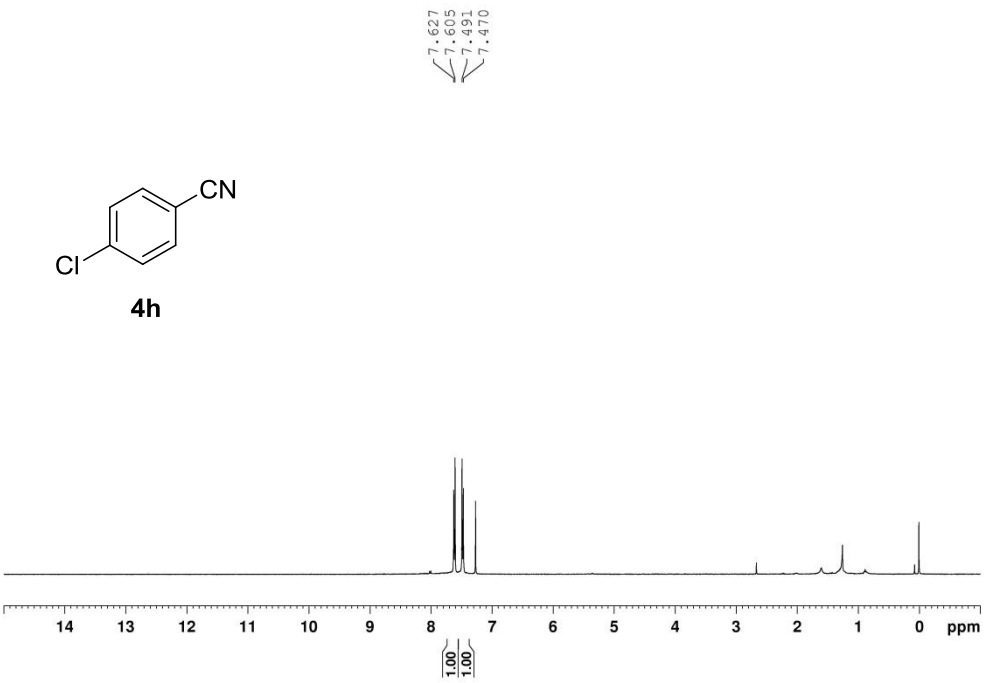

CN
HO

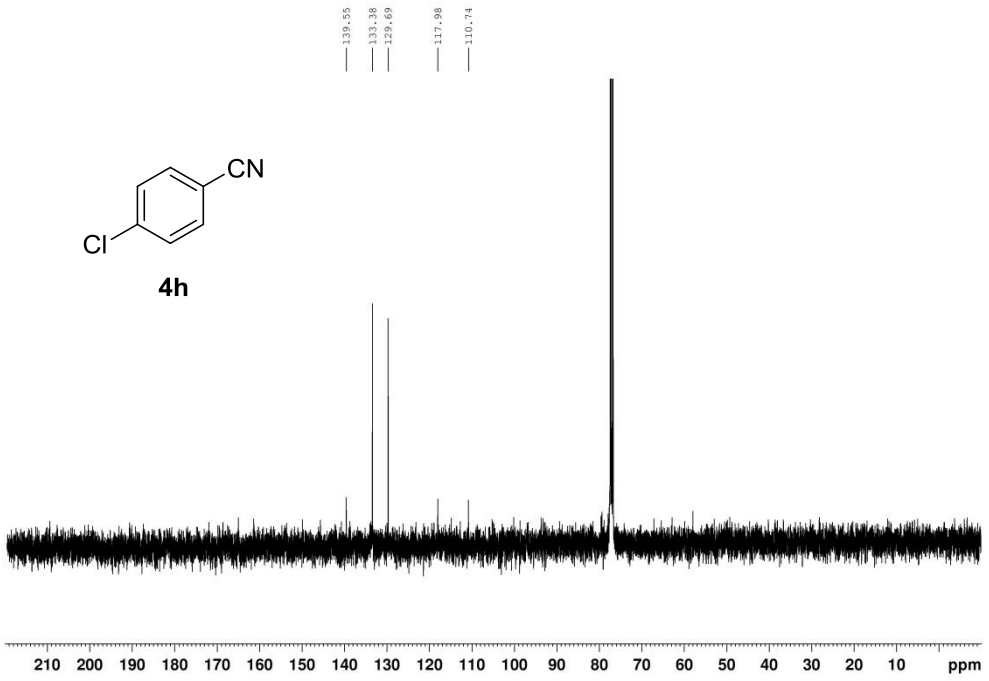
4f

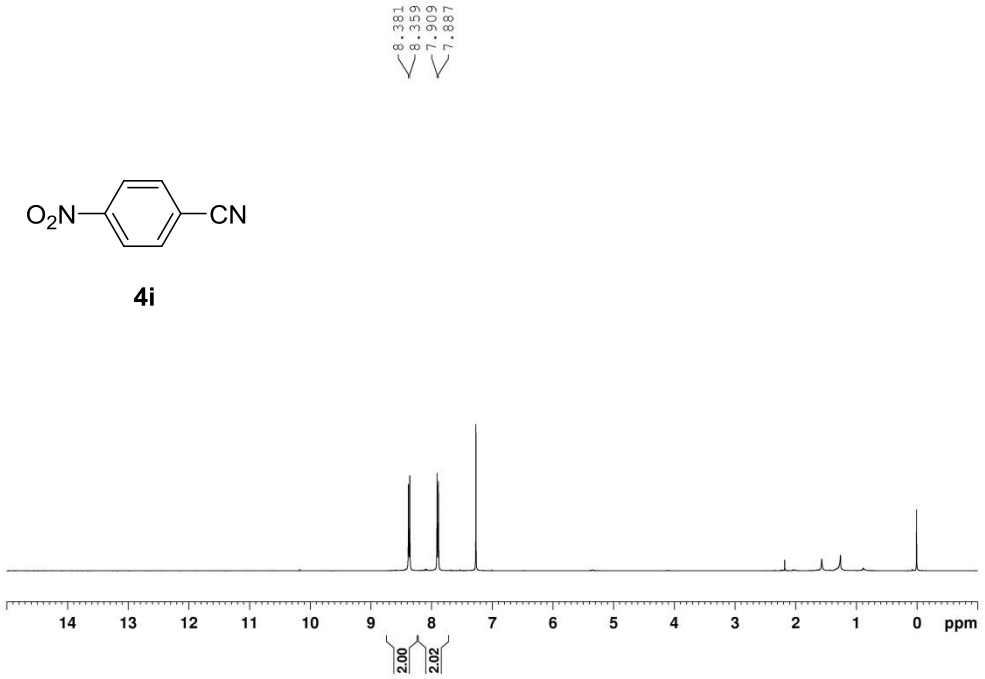

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

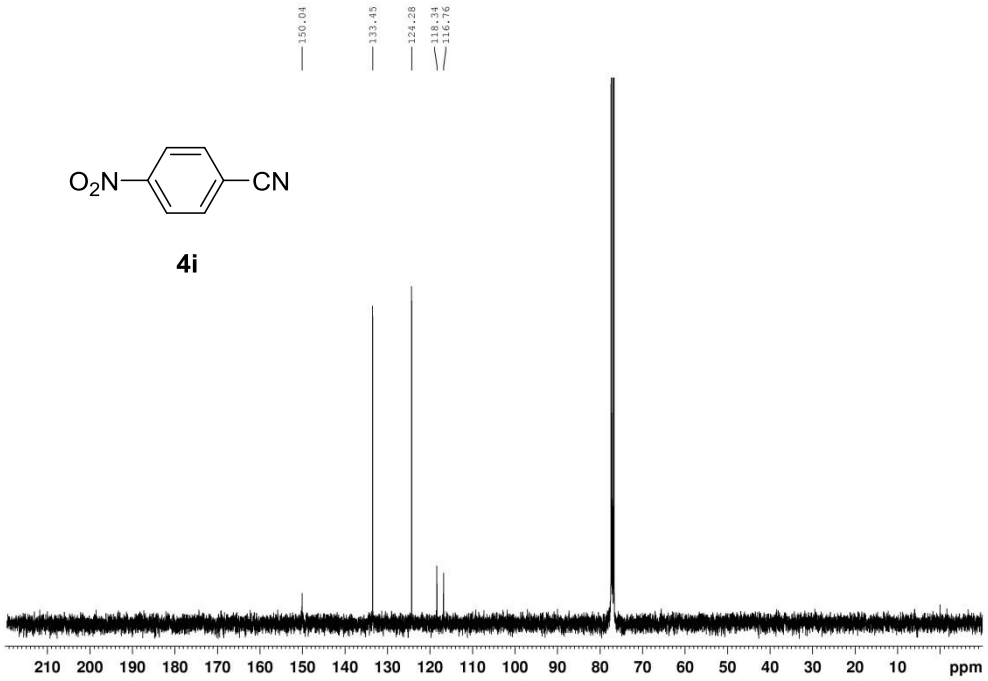

7.655
7.634
7.545
7.524
CN
Br
4g
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.00
2.01

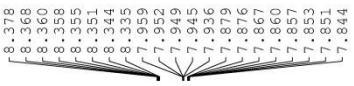

133.38
132.61
128.00
118.05
111.18
CN
Br
4g
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

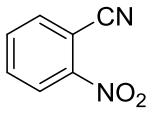

7.627
7.605
7.491
7.470
CN
Cl
4h
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
1.00


139.55
133.38
129.69
117.98
110.74
CN
Cl
4h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

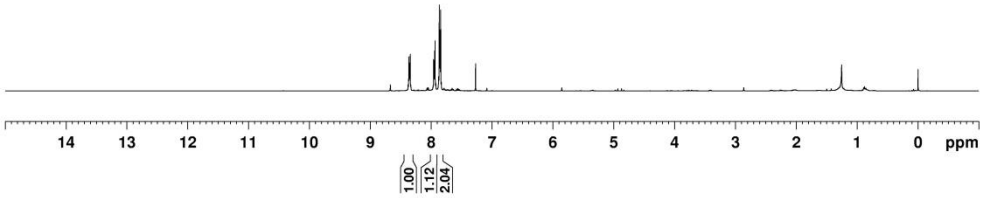

8.381
8.359
7.909
7.887
O2N
CN
4i
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.00
2.02


150.04
133.45
124.28
118.34
116.76
O2N
CN
4i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

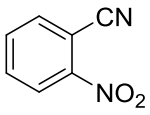

8.378
8.368
8.360
8.358
8.355
8.351
8.344
8.335
7.959
7.952
7.949
7.945
7.936
7.879
7.876
7.867
7.860
7.857
7.853
7.851
7.844


CN
NO2

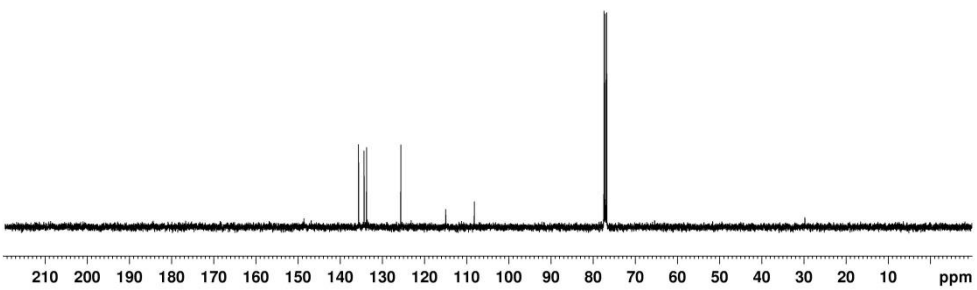
4j

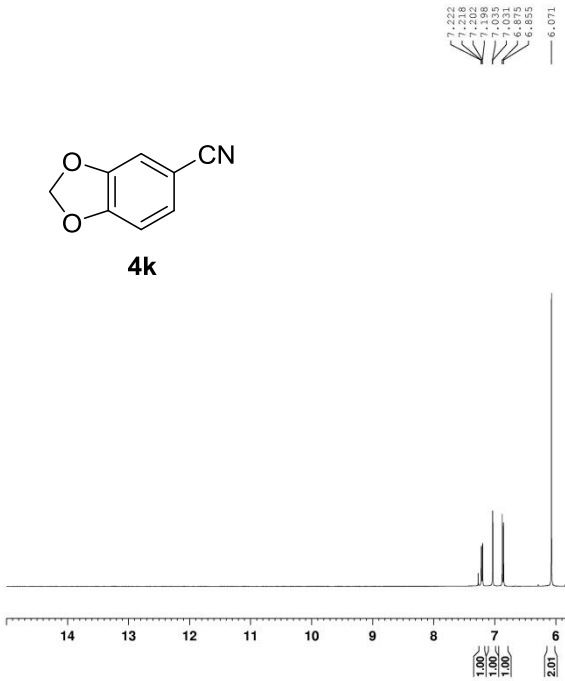

14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.12
2.04


135.57
134.72
133.66
125.53
114.89
108.08

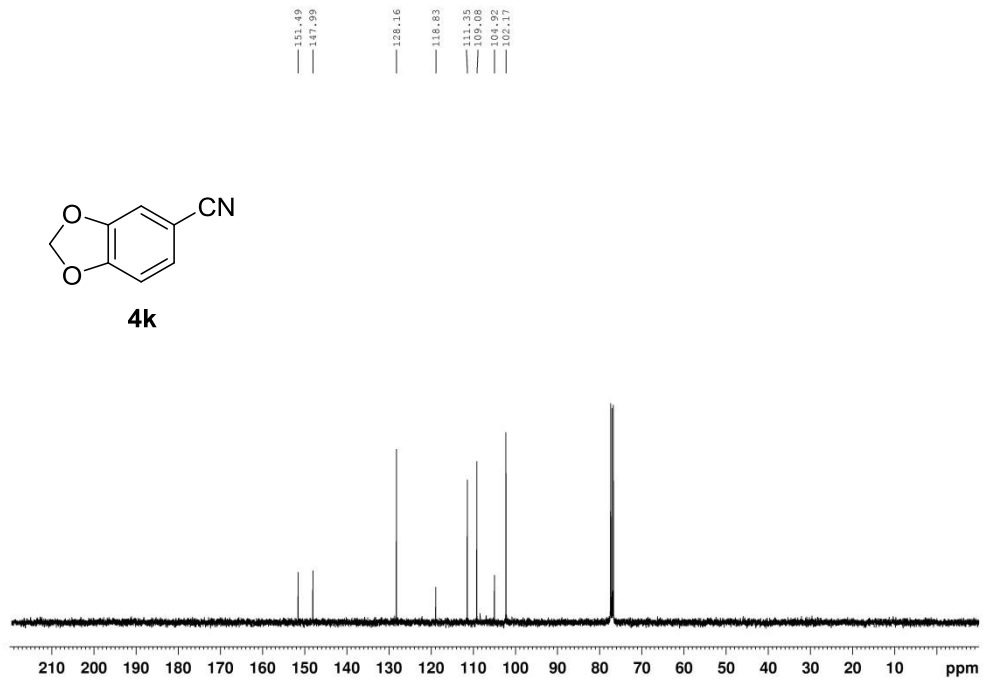

CN
NO2

4j

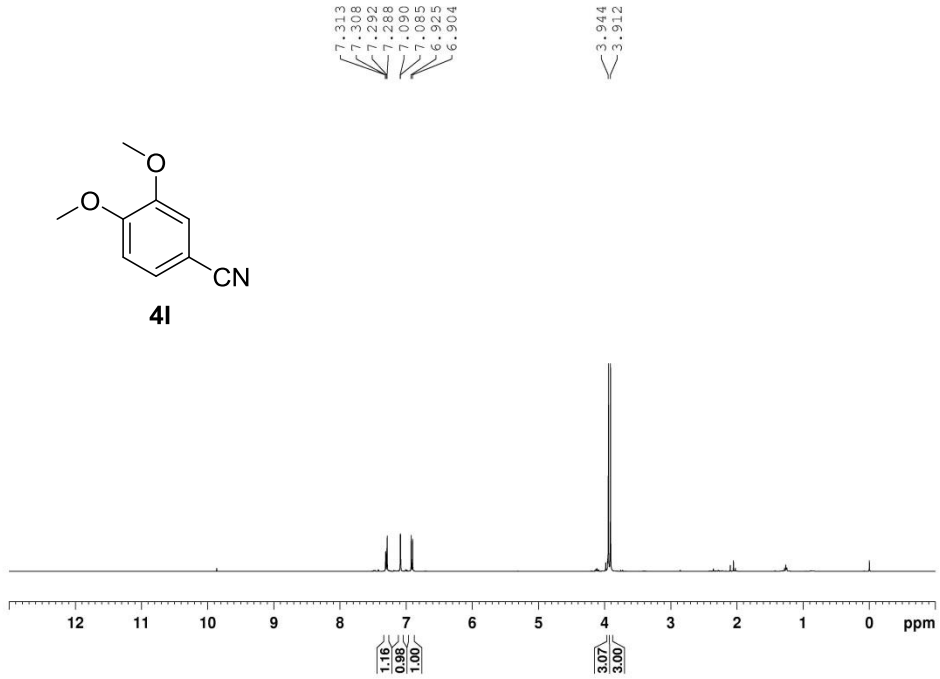

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

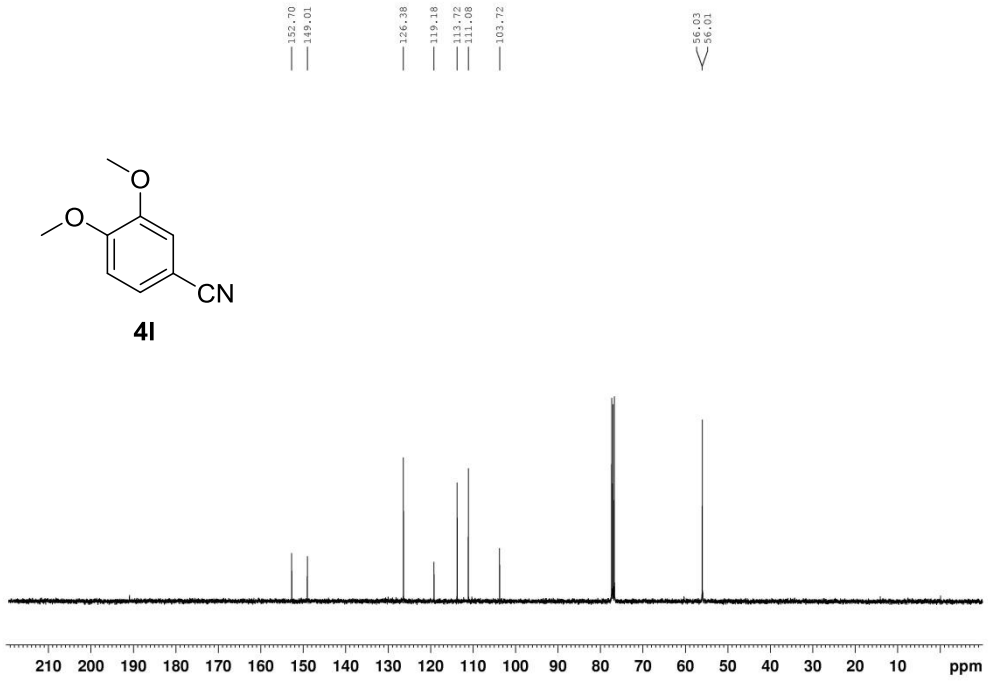

7.222
7.218
7.202
7.198
7.035
7.031
6.875
6.855
6.071
CN
O
O
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.00
1.00
2.01

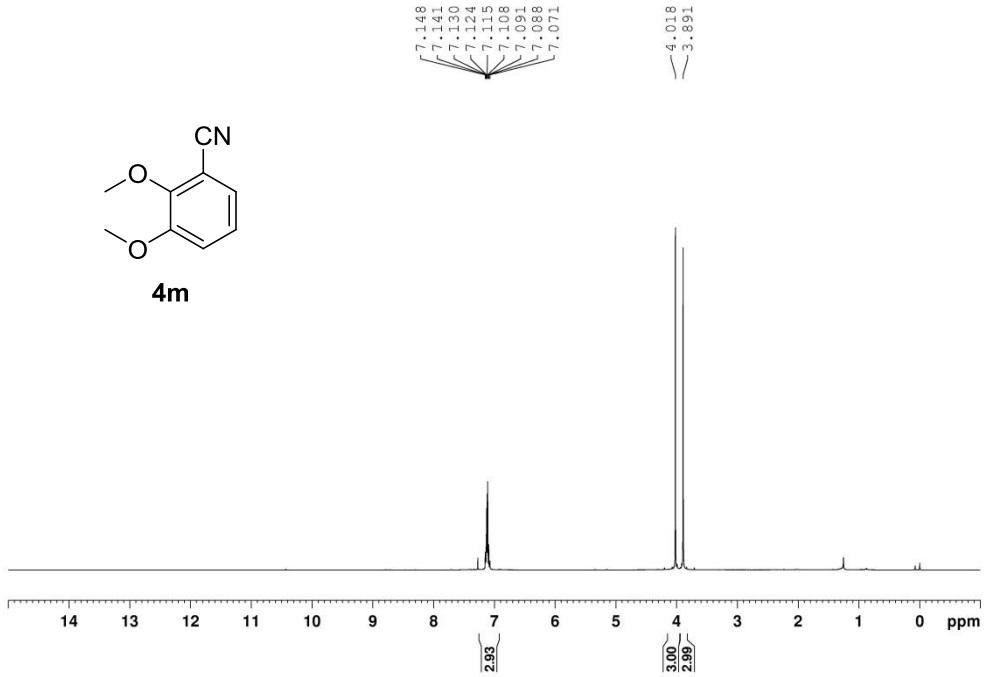
4k

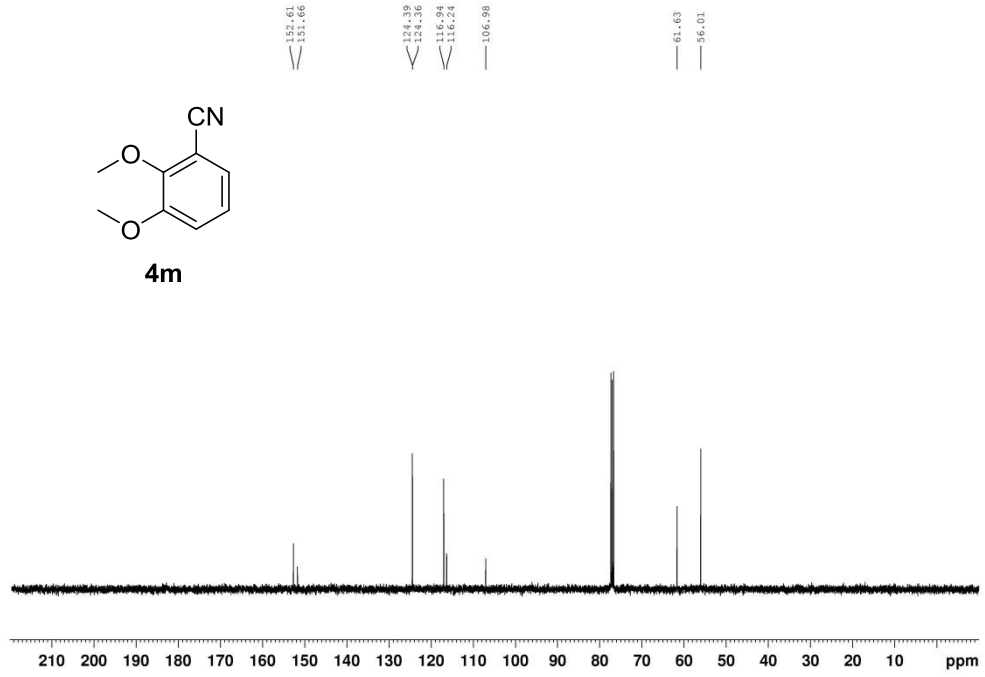

151.49
147.99
128.16
118.83
111.35
109.08
104.92
102.17
CN
O
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

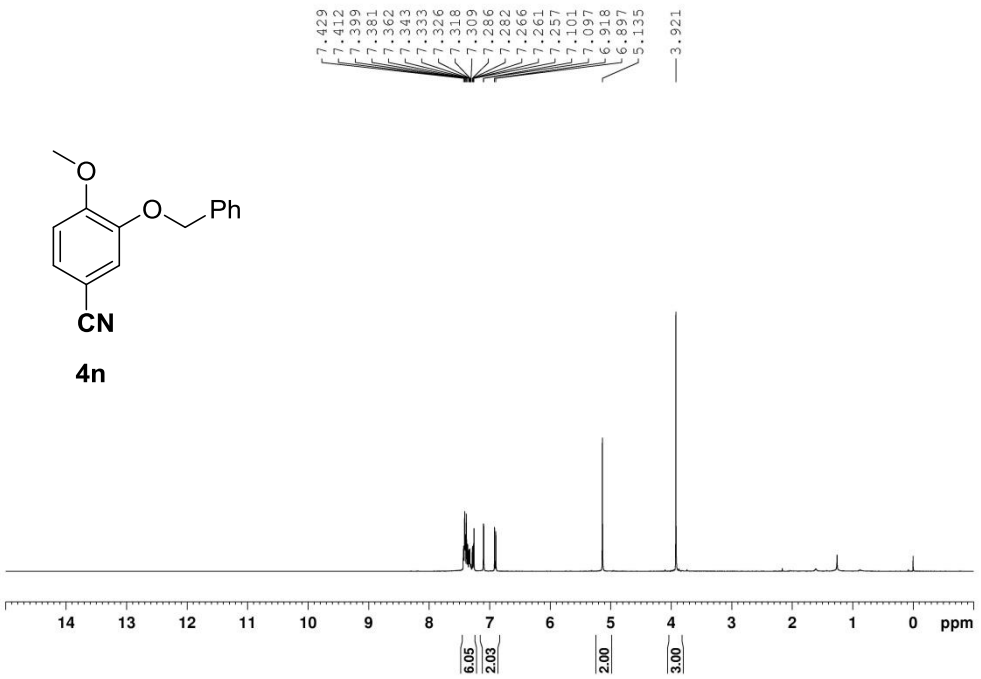
4k

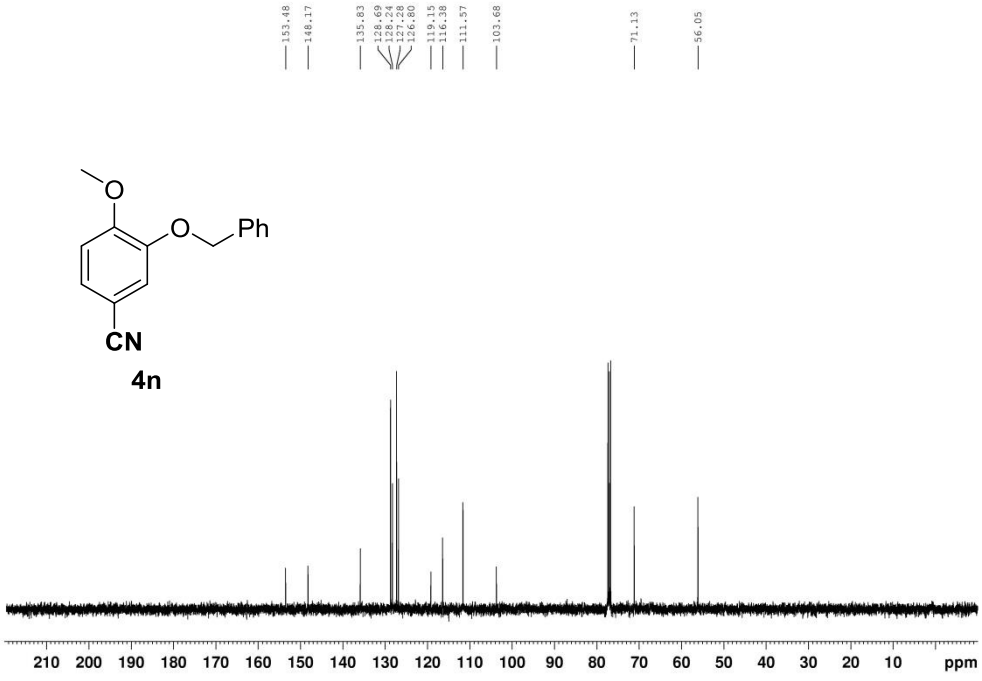

7.313
7.308
7.292
7.288
7.090
7.085
6.925
6.904
3.944
3.912
O
O
CN
4l
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.16
0.98
1.00
3.07
3.00

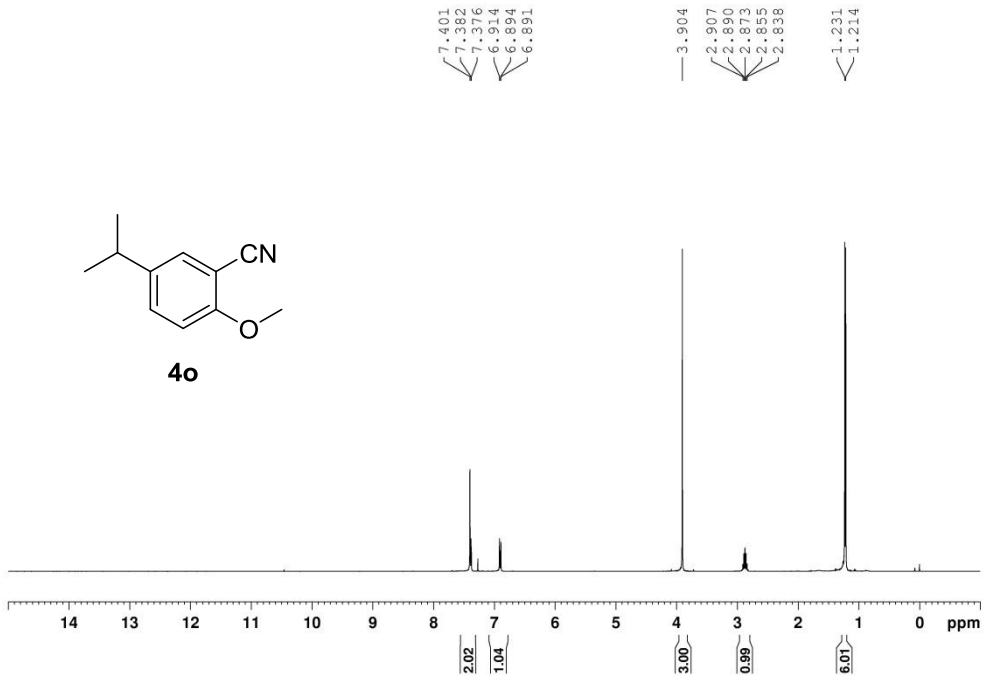

152.70
149.01
126.38
119.18
113.72
111.08
103.72
56.03
56.01
O
O
CN
4l
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

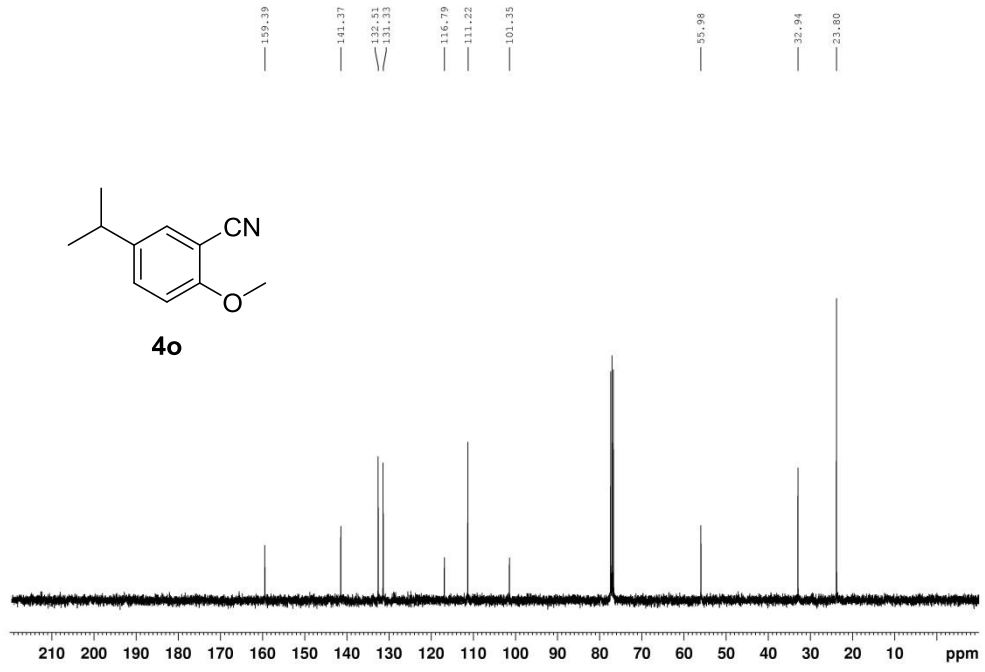

7.148
7.141
7.130
7.124
7.115
7.108
7.091
7.088
7.071
4.018
3.891
CN
O
O
4m
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.93
3.00
2.99

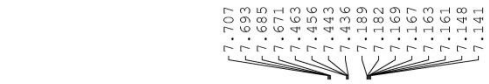

152.61
151.66
124.39
124.36
116.94
116.24
106.98
61.63
56.01
CN
O
O
4m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

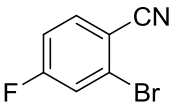

7.429
7.412
7.399
7.381
7.362
7.343
7.333
7.326
7.318
7.309
7.286
7.282
7.266
7.261
7.257
7.101
7.097
6.918
6.897
5.135
3.921
O
O
Ph
CN
4n
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
6.05
2.03
2.00
3.00


153.48
148.17
135.83
128.69
128.24
127.28
126.80
119.15
116.38
111.57
103.68
71.13
56.05
O
O
Ph
CN
4n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

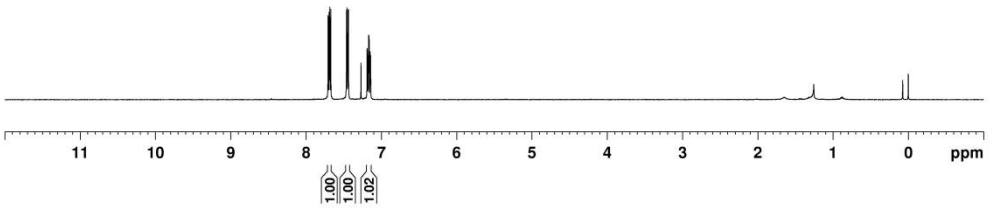

7.401
7.382
7.376
6.914
6.894
6.891
3.904
2.907
2.890
2.873
2.855
2.838
1.231
1.214
CN
O
4o
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.02
1.04
3.00
0.99
6.01


159.39
141.37
132.51
131.33
116.79
111.22
101.35
55.98
32.94
23.80
CN
O
4o
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

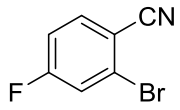

7.707
7.693
7.685
7.671
7.463
7.456
7.443
7.436
7.189
7.182
7.169
7.167
7.163
7.161
7.148
7.141


CN
F
Br

4p

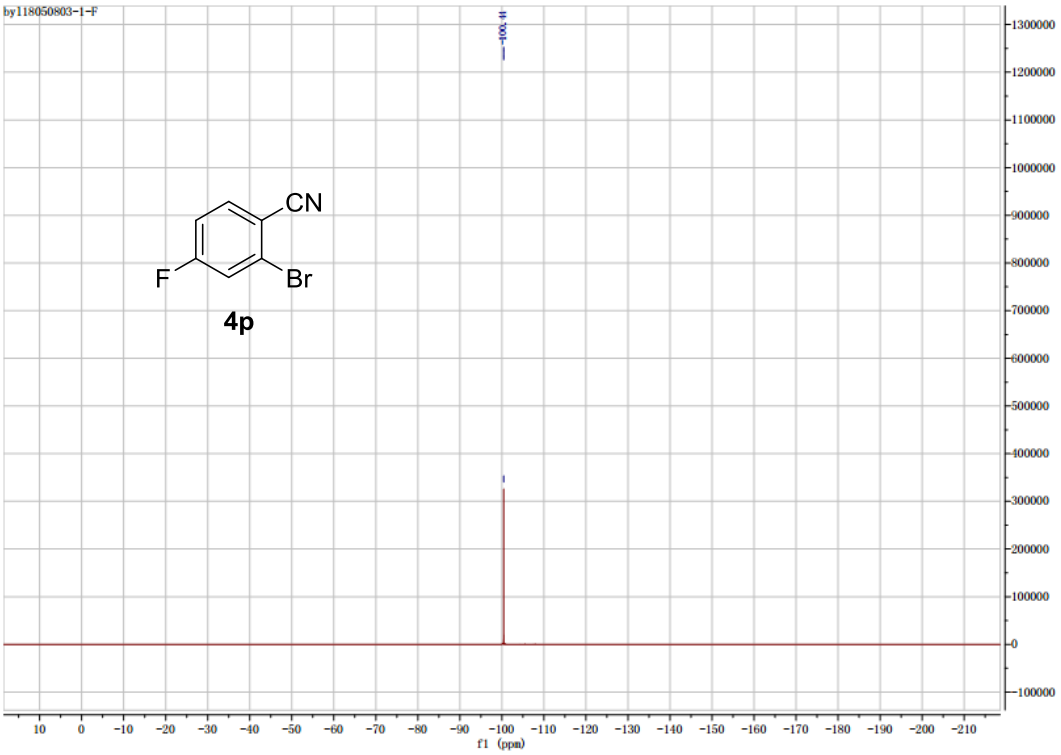

11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.00
1.02


165.77
163.18
136.03
135.94
126.77
126.67
121.33
121.08
116.42
115.77
115.55
112.30
112.26

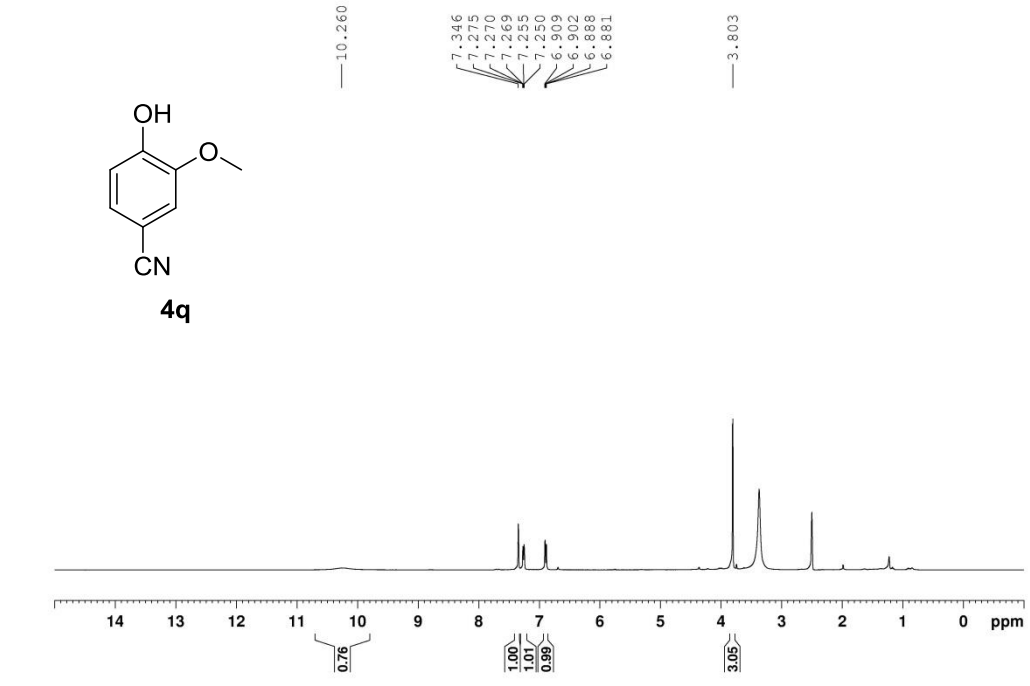

CN
F
Br

4p

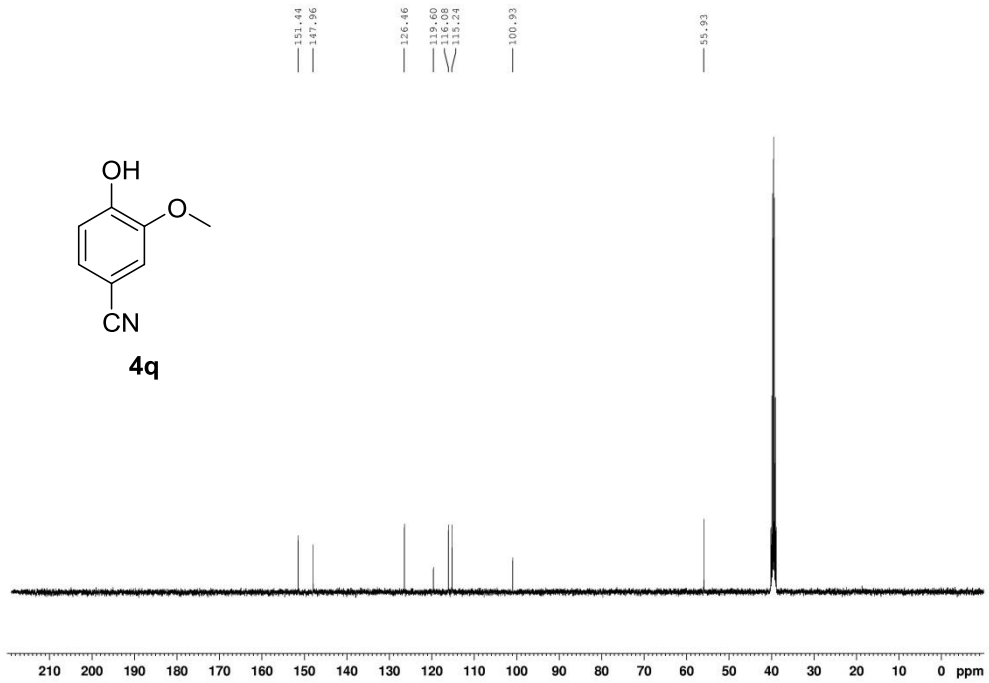
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


by118050803-1-F
CN
F
Br
f1 (ppm)

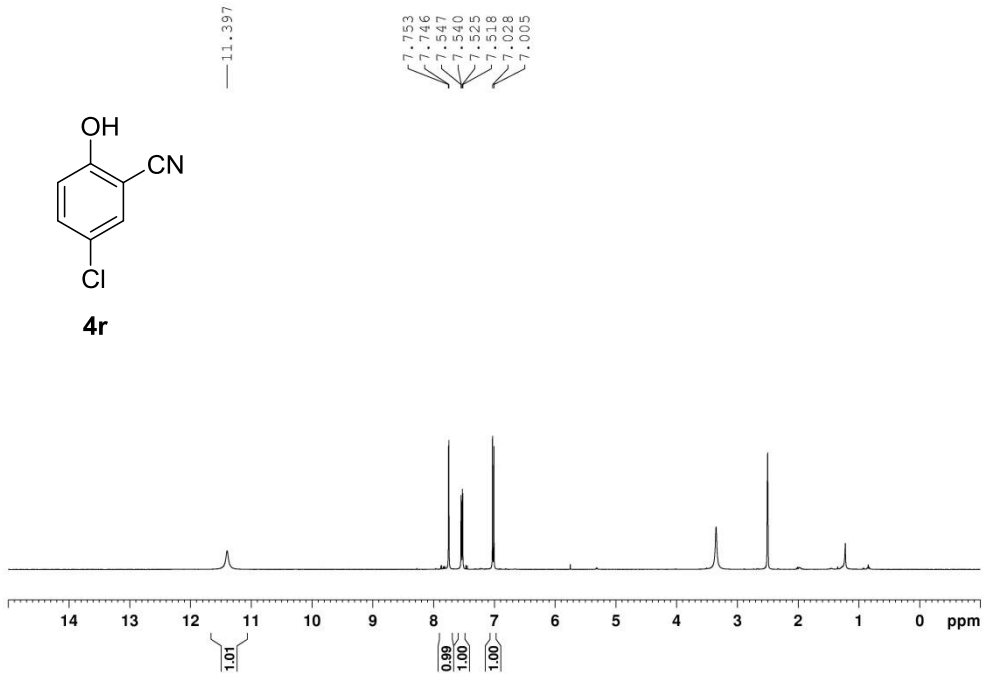
4p


10.260
7.346
7.275
7.270
7.269
7.255
7.250
6.909
6.902
6.888
6.881
3.803
OH
O
CN
ppm
0.76
1.00
1.01
0.99
3.05

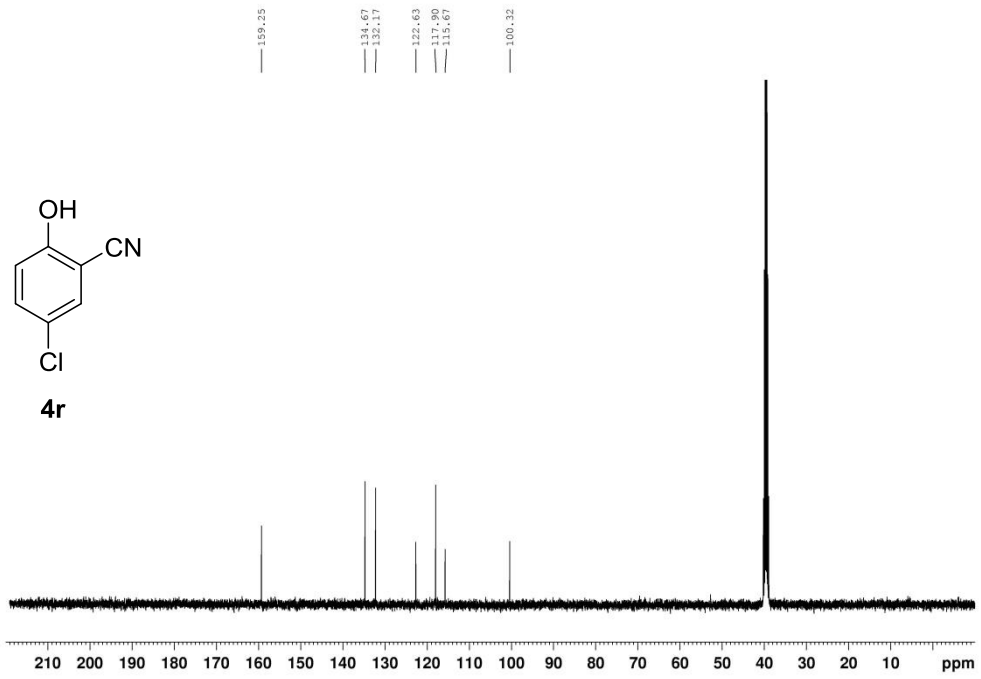
4q

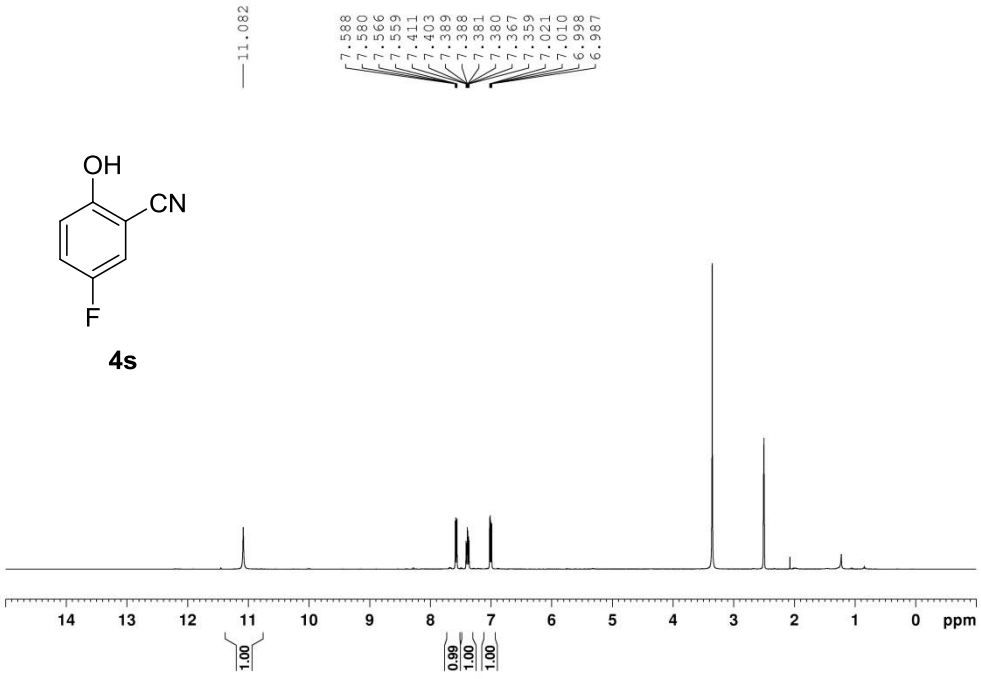

151.44
147.96
126.46
119.60
116.08
115.24
100.93
55.93
OH
O
CN
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

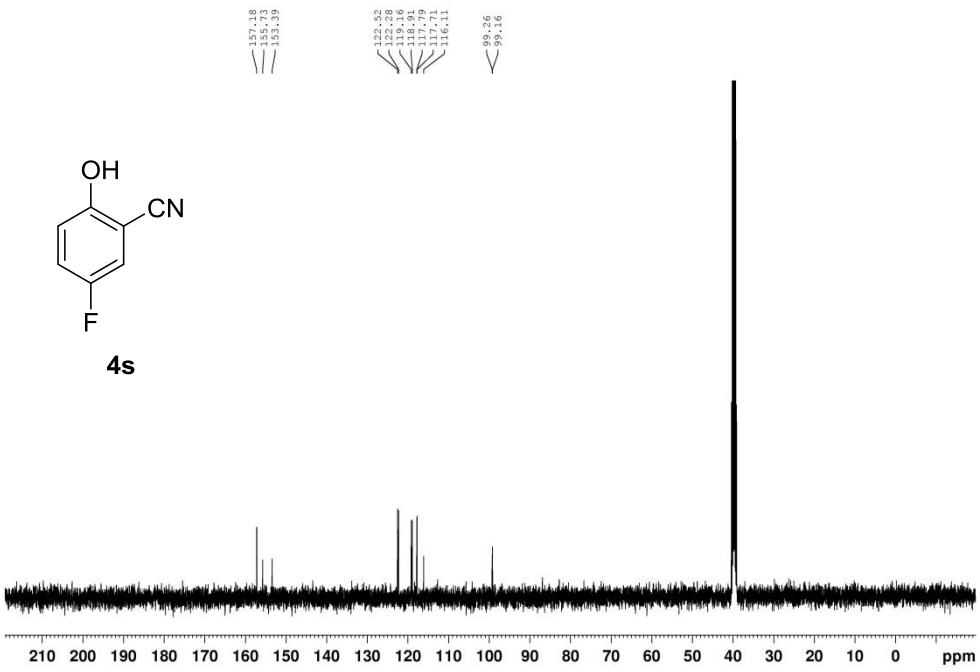
4q

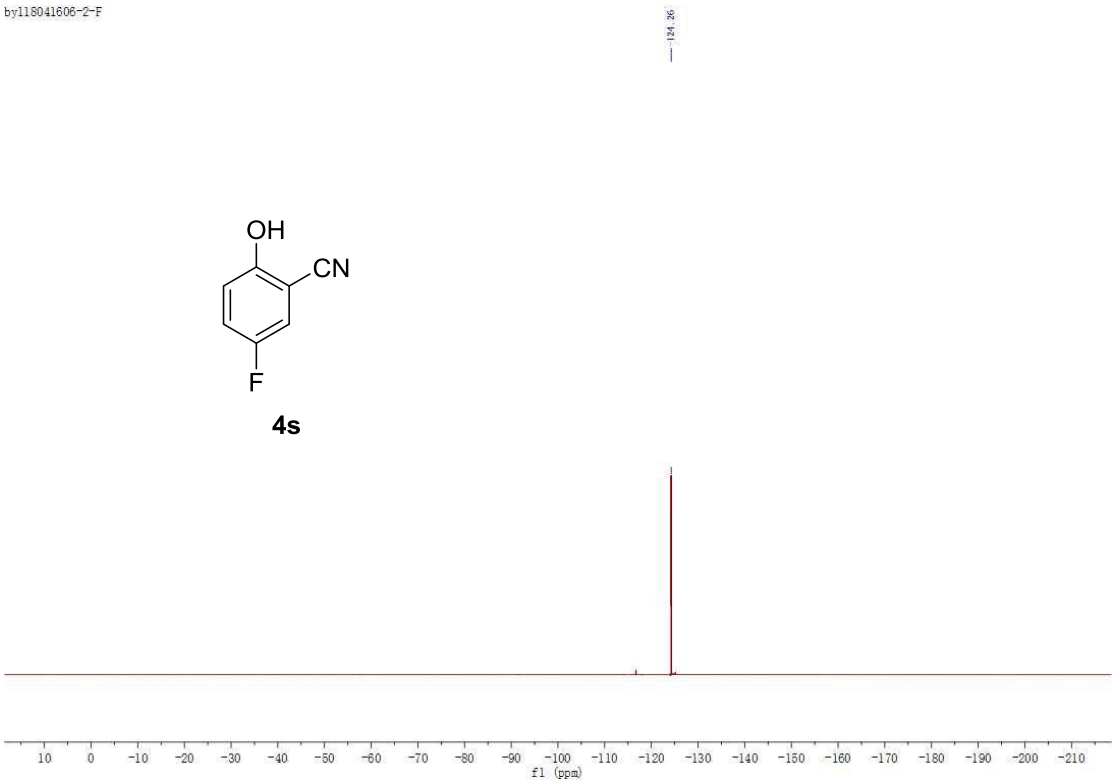

11.397
7.753
7.746
7.547
7.540
7.525
7.518
7.028
7.005
OH
CN
Cl
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.01
0.99
1.00
1.00

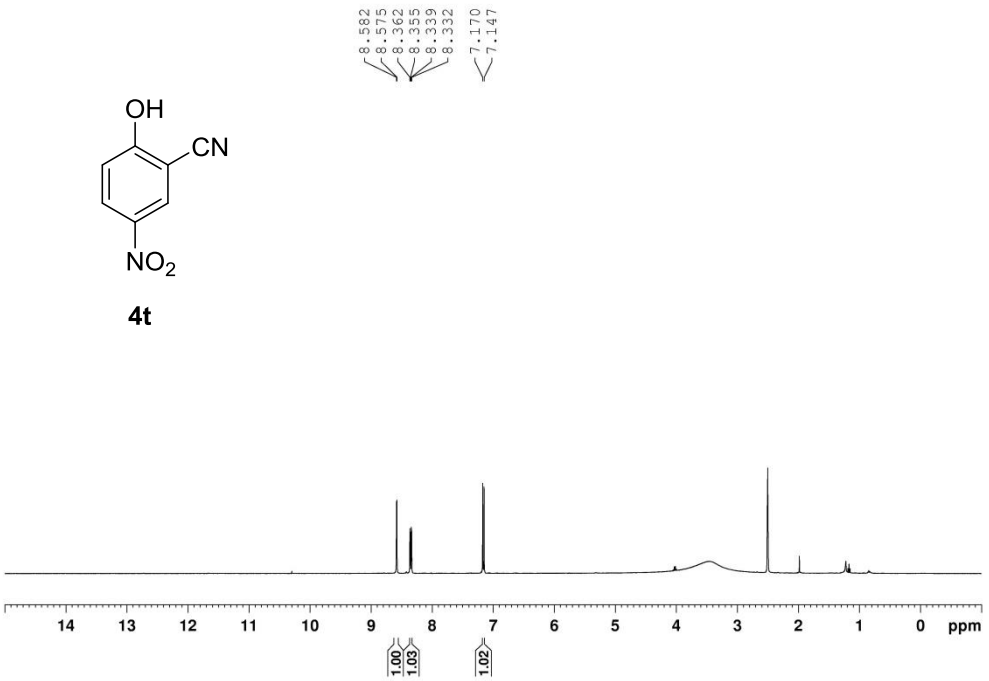
4r

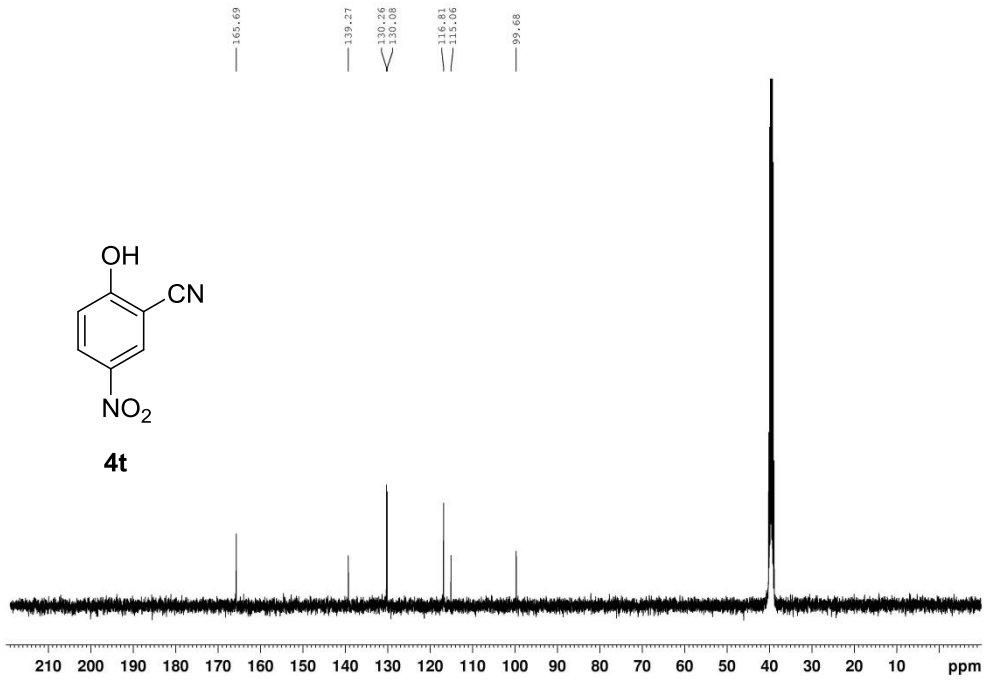

159.25
134.67
132.17
122.63
117.90
115.67
100.32
OH
CN
Cl
4r
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

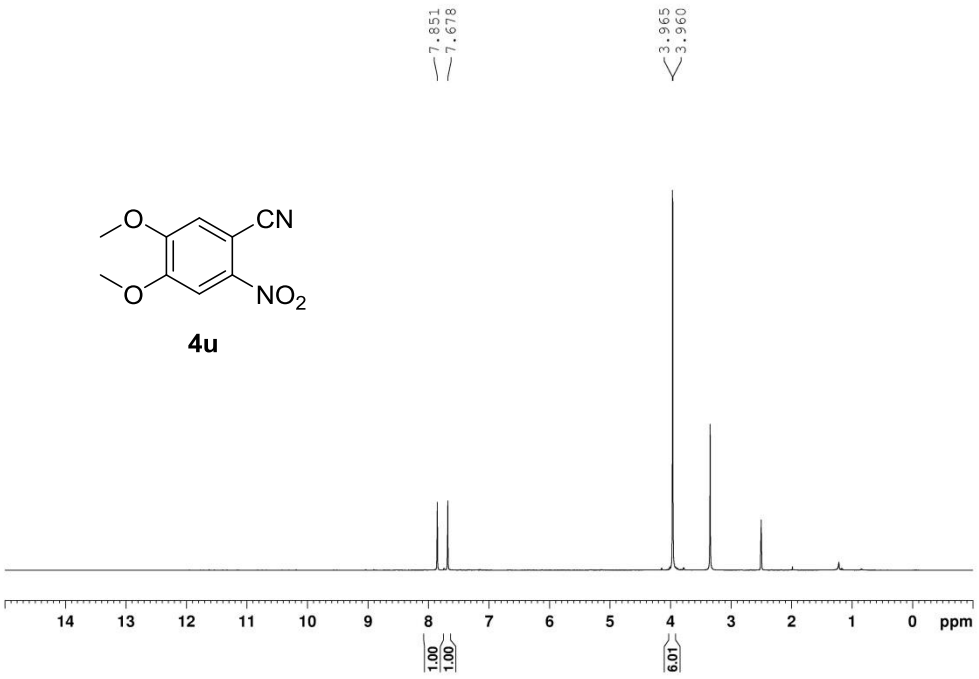

11.082
7.588
7.580
7.566
7.559
7.411
7.403
7.389
7.388
7.381
7.380
7.367
7.359
7.021
7.010
6.998
6.987
OH
CN
F
4s
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
0.99
1.00
1.00

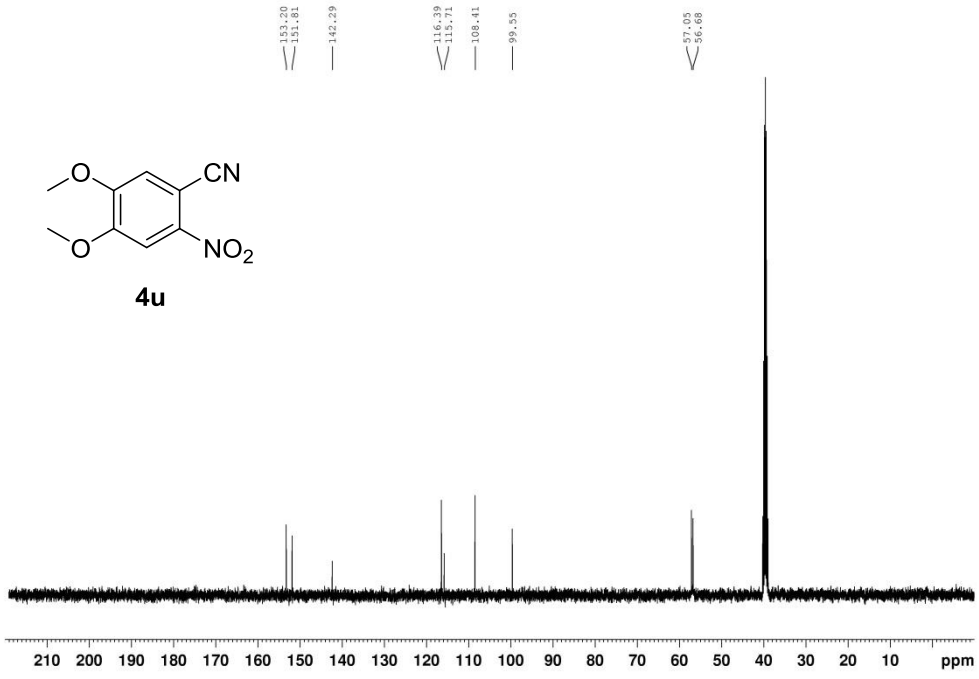

157.18
155.73
153.39
122.52
122.28
119.16
118.91
118.69
117.71
116.11
99.26
99.16
OH
CN
F
4s
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

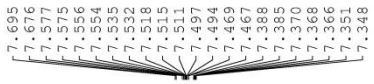

by118041606-2-F
-124.26
OH
CN
F
4s
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

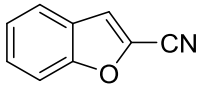

8.582
8.575
8.362
8.355
8.339
8.332
7.170
7.147
OH
CN
NO2
4t
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
1.03
1.02


165.69
139.27
130.26
130.08
116.81
115.06
99.68
OH
CN
NO2
4t
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

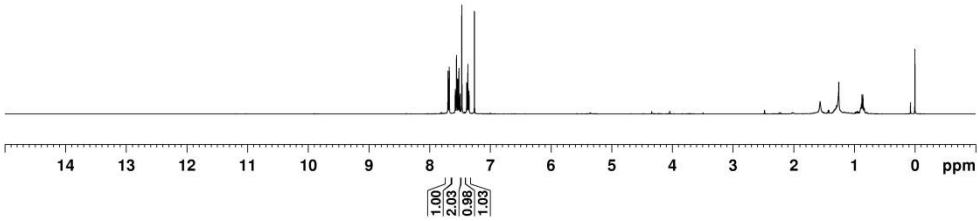

7.851
7.678
3.965
3.960
CN
O
O
NO2
4u
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
1.00
6.01


153.20
151.81
142.29
116.39
115.71
108.41
99.55
57.05
56.68
CN
O
O
NO2
4u
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

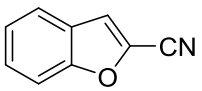

7.695
7.676
7.577
7.575
7.556
7.554
7.535
7.532
7.518
7.515
7.511
7.497
7.494
7.469
7.467
7.388
7.385
7.370
7.368
7.366
7.351
7.348


CN
O

4v

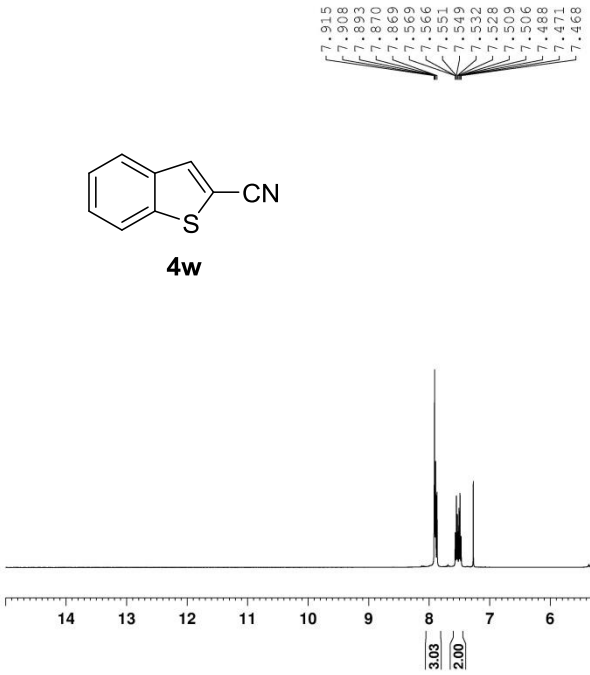

14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
2.03
0.98
1.03

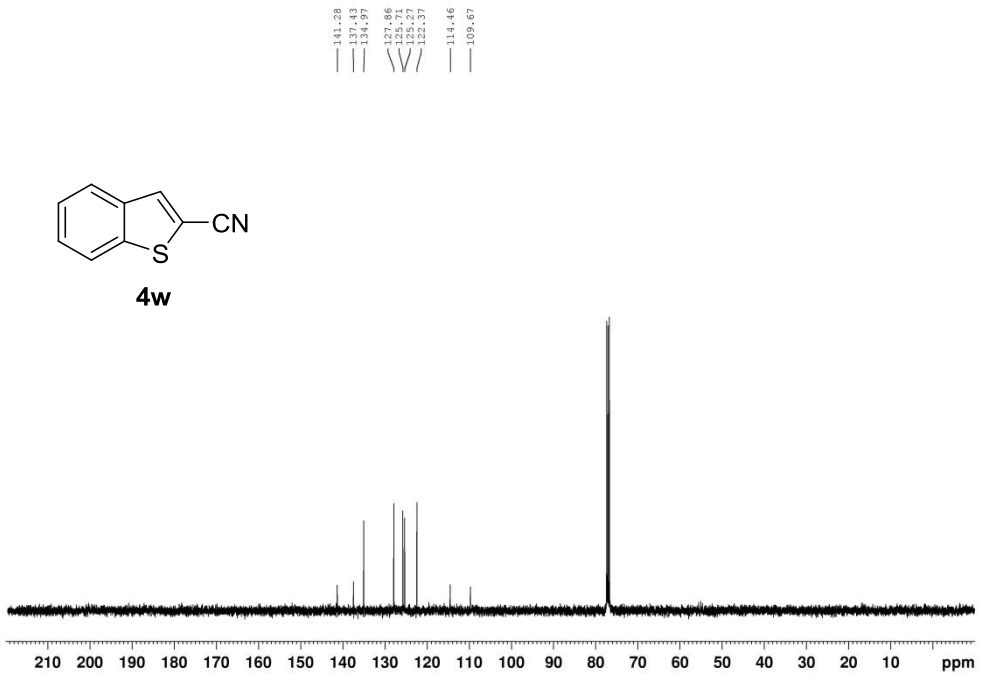

155.68
128.43
127.33
125.49
124.55
122.56
118.44
112.11
111.82

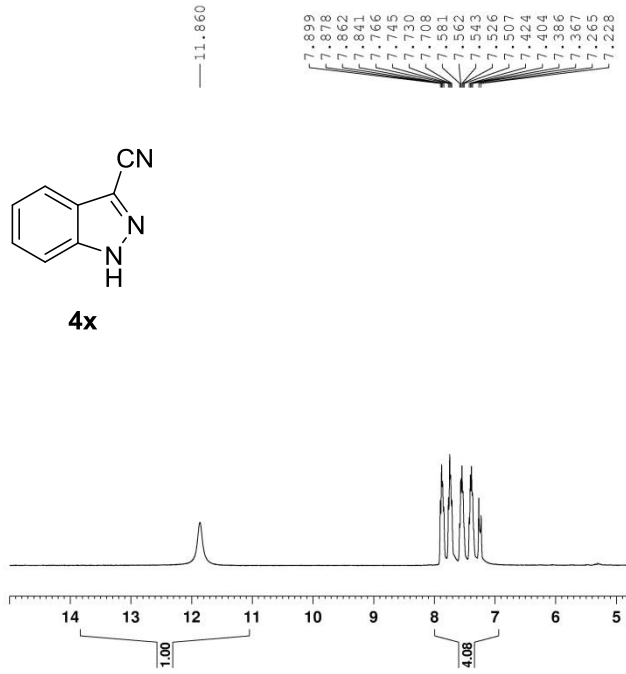

CN
O

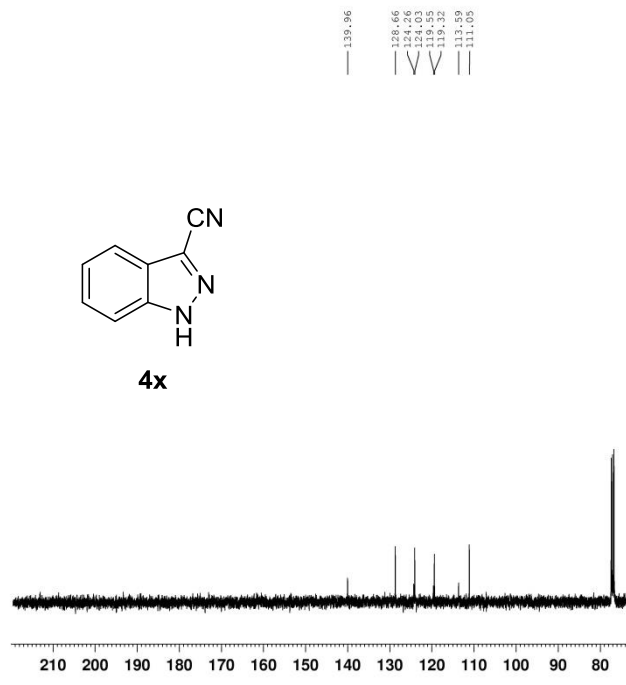
4v

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

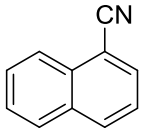

7.915
7.908
7.893
7.870
7.869
7.569
7.566
7.551
7.549
7.532
7.528
7.509
7.506
7.488
7.471
7.468
CN
S
4w
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
3.03
2.00


141.28
137.43
134.97
127.86
125.71
125.37
122.37
114.46
109.67
CN
S
4w
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

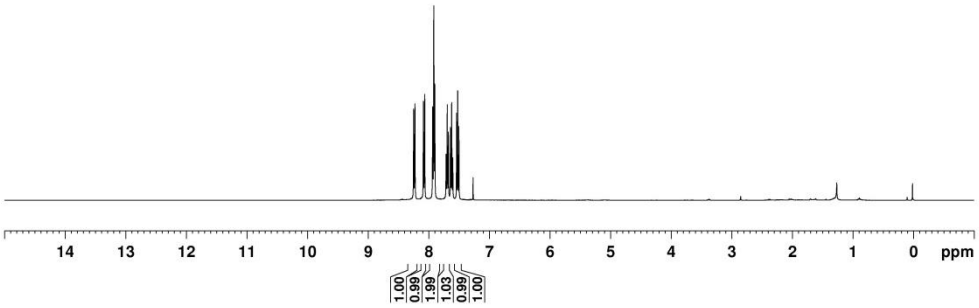

11.860
7.899
7.878
7.862
7.841
7.766
7.745
7.730
7.708
7.581
7.562
7.543
7.526
7.507
7.424
7.404
7.386
7.367
7.265
7.228
CN
N
N
H
4x
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
4.08

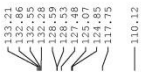

139.96
128.66
124.26
124.03
119.55
119.32
113.59
111.05
CN
N
N
H
4x
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

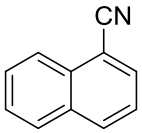

8.251
8.230
8.090
8.069
7.937
7.918
7.903
7.900
7.717
7.714
7.699
7.697
7.679
7.676
7.644
7.641
7.624
7.606
7.604
7.543
7.524
7.522
7.504


CN

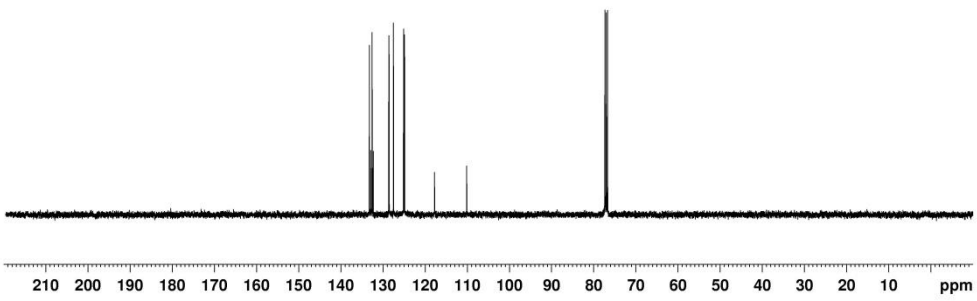
4y


14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
0.99
1.99
1.03
0.99
1.00

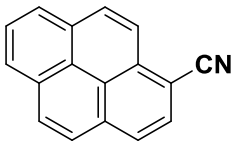

133.21
132.66
132.55
132.28
128.59
128.33
127.48
125.07
124.85
117.75
110.12


CN

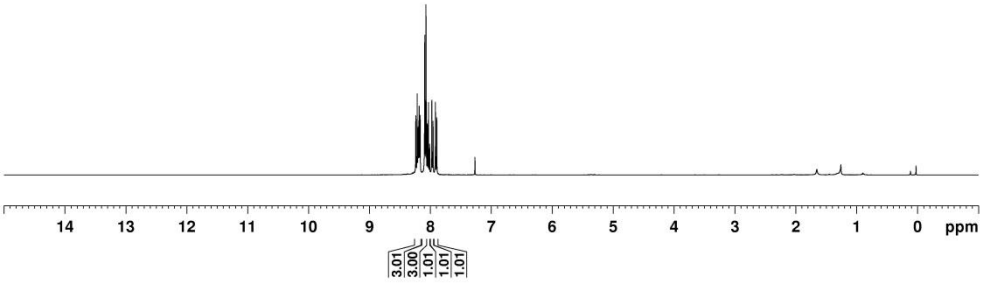
4y

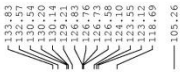

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

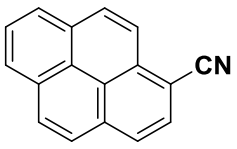

8.241
8.218
8.202
8.186
8.170
8.094
8.074
8.052
8.033
8.014
7.978
7.958
7.919
7.897


CN

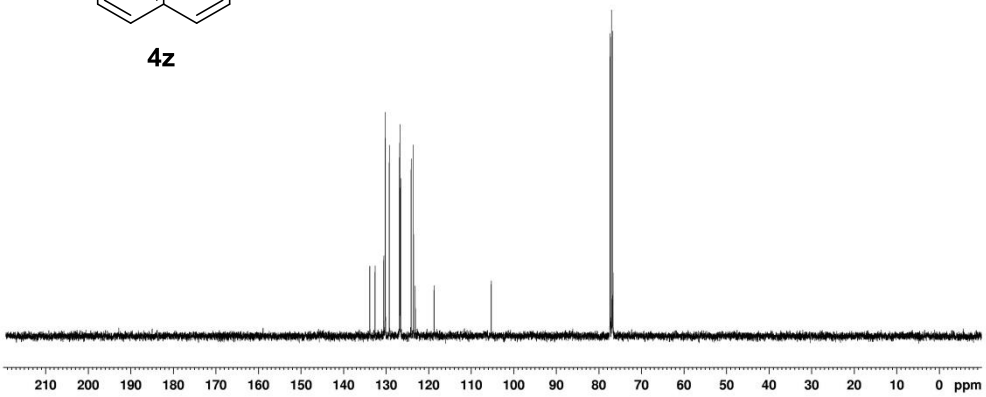
4z

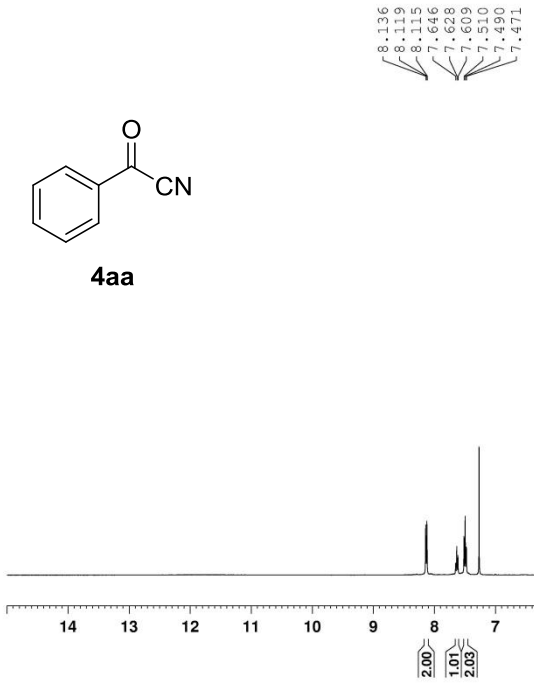

14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
3.01
3.00
1.01
1.01
1.01

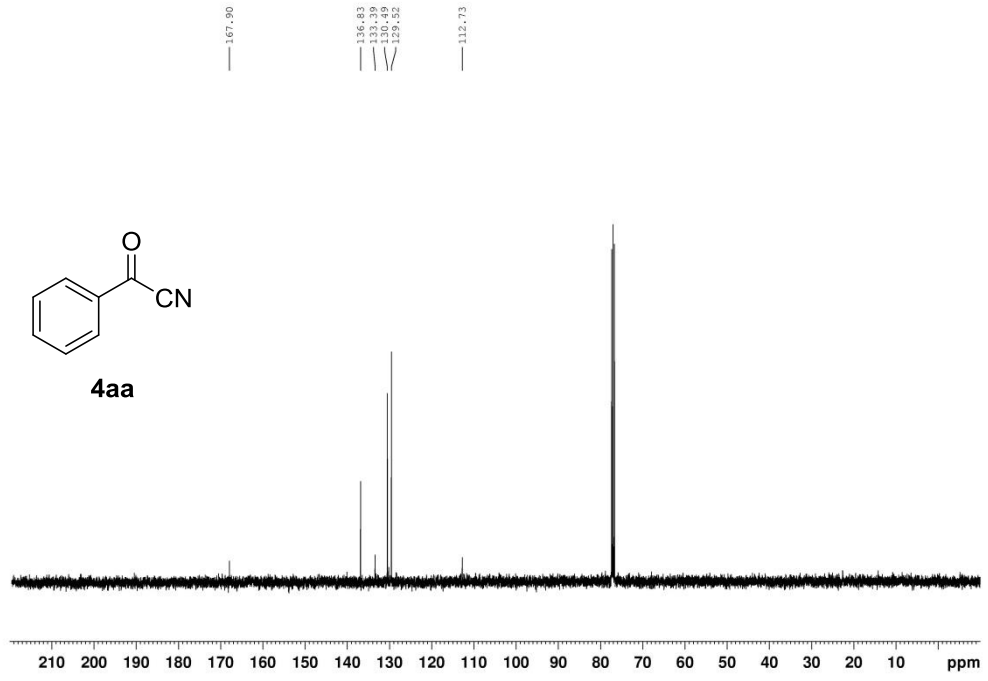

133.83
132.57
130.54
130.20
130.14
129.31
126.83
126.76
126.73
126.18
124.10
123.55
123.12
118.69
105.26


CN

4z


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


8.136
8.119
8.115
7.646
7.628
7.609
7.510
7.490
7.471
O
CN
4aa
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.00
1.01
2.03


167.90
136.83
133.39
130.49
129.52
112.73
O
CN
4aa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm