Supporting Information

Facile access to 2-acyloxy-, aryloxy- and enyloxy-2*H*-azirines via an S_N2'-S_N2' cascade in 2-halo-2*H*-azirines

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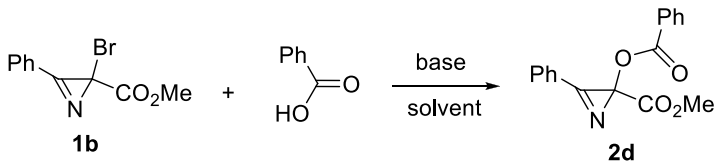
Contents

1. Table S-1. Optimization of reaction conditions [a]



entry	solvent	base	time, h [b]	yield of **2d**, % [c]
1	PhMe	–	100	no reaction
2	PhMe	NEt_3	2	88
3	PhMe	DBU	2	0
4	PhMe	Pyridine	2	0
5	acetone	NEt_3	2	77
6	CH_3CN	NEt_3	2	69
7	CH_2Cl_2	NEt_3	2	80
8	THF	NEt_3	2	72
9	CH_3OH	NEt_3	3	13[d]
10[e]	PhMe	NEt_3	4	89

[a] Reaction conditions: **1b** (0.04 mmol), benzoic acid (0.06 mmol), base (0.18 mmol), solvent (0.5 mL), r.t.

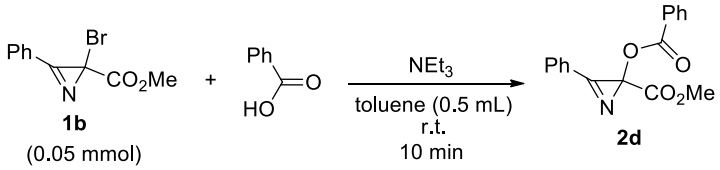
[b] Time after which starting bromoazirine **1b** was fully consumed according to TLC.

[c] ^{1}H NMR yields using CH_2Br_2 as an internal standard.

[d] Methyl 2-methoxy-3-phenyl-2*H*-azirine-2-carboxylate (**7f**) was also formed (^{1}H NMR yield is 28%).

[e] Reaction conditions: **1b** (0.04 mmol), benzoic acid (0.048 mmol) and NEt_3 (0.08 mmol), PhMe (0.5 mL), r.t.

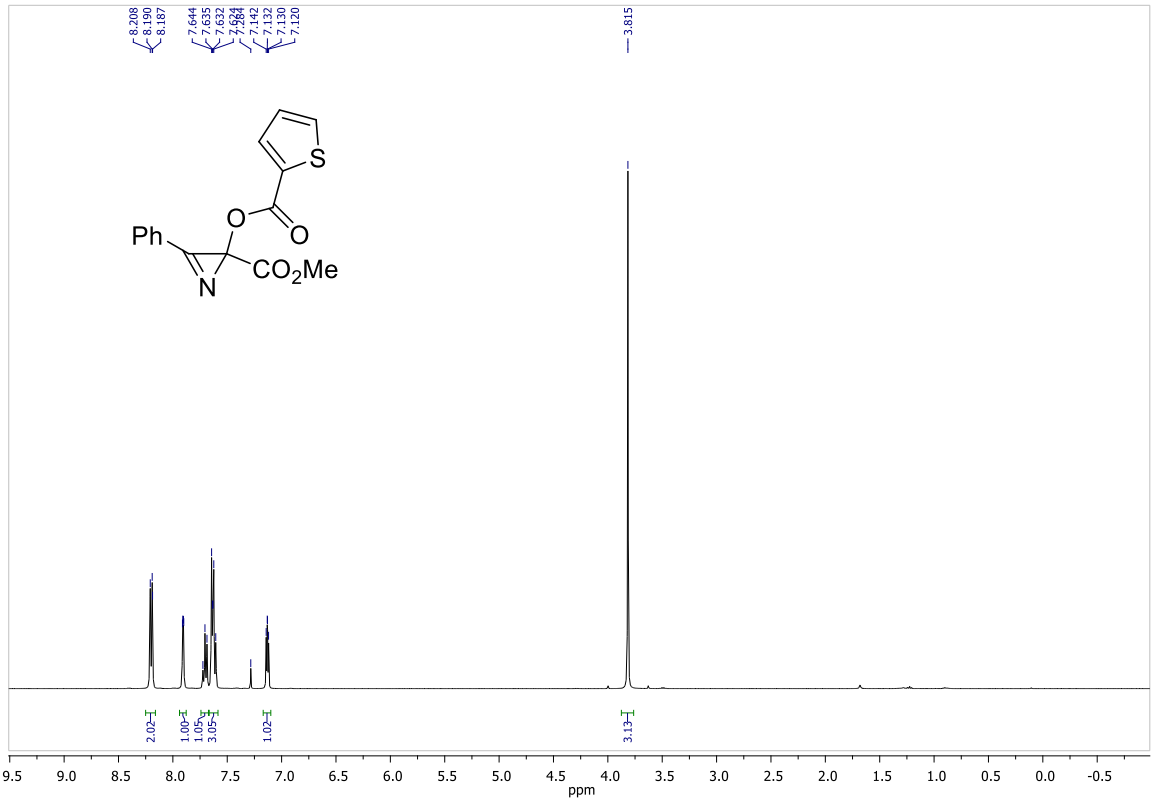
2. Table S-2. Consumption of azirine **1b** after 10 min, depending on the used amount of benzoic acid and Et_3N

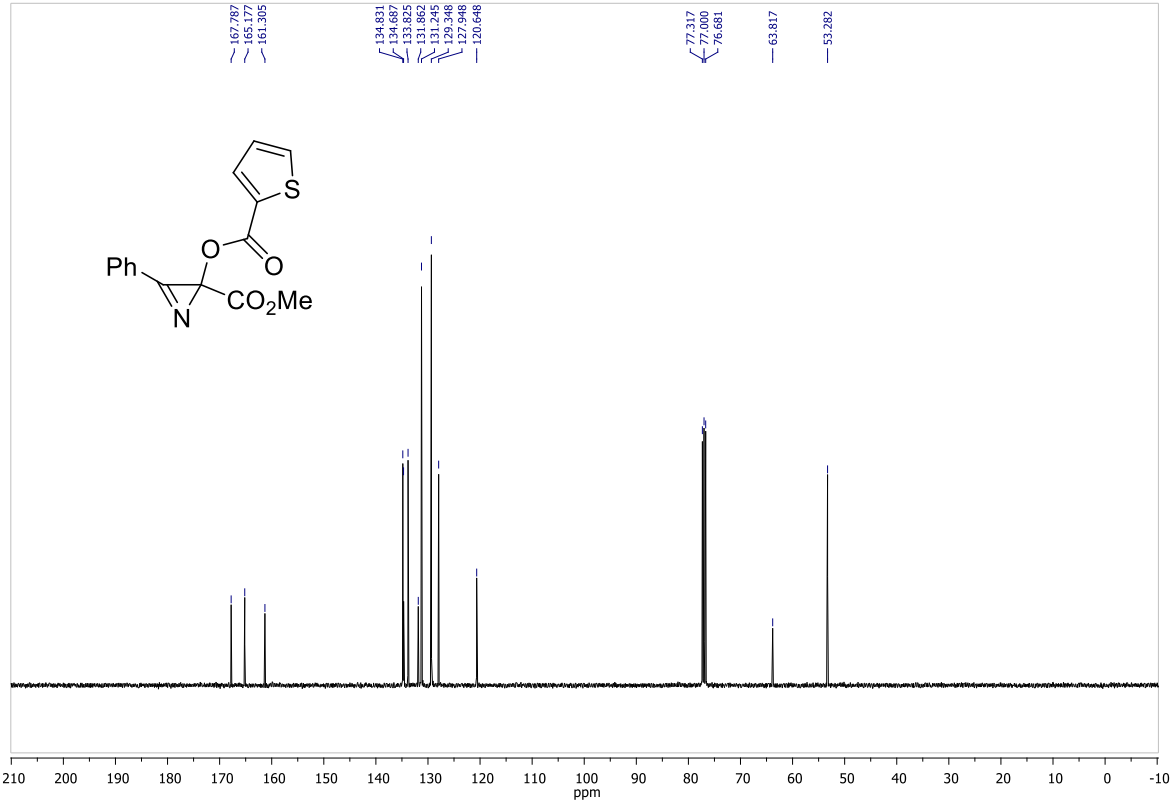


Entry	Benzoic acid	NEt_3	Conversion of **1b**, % (^{1}H NMR)
1	0.06 mmol (1.2 equiv)	0.1 mmol (2 equiv)	56
2	0.06 mmol (1.2 equiv)	0.2 mmol (4 equiv)	56
3	0.12 mmol (2.4 equiv)	0.2 mmol (4 equiv)	81

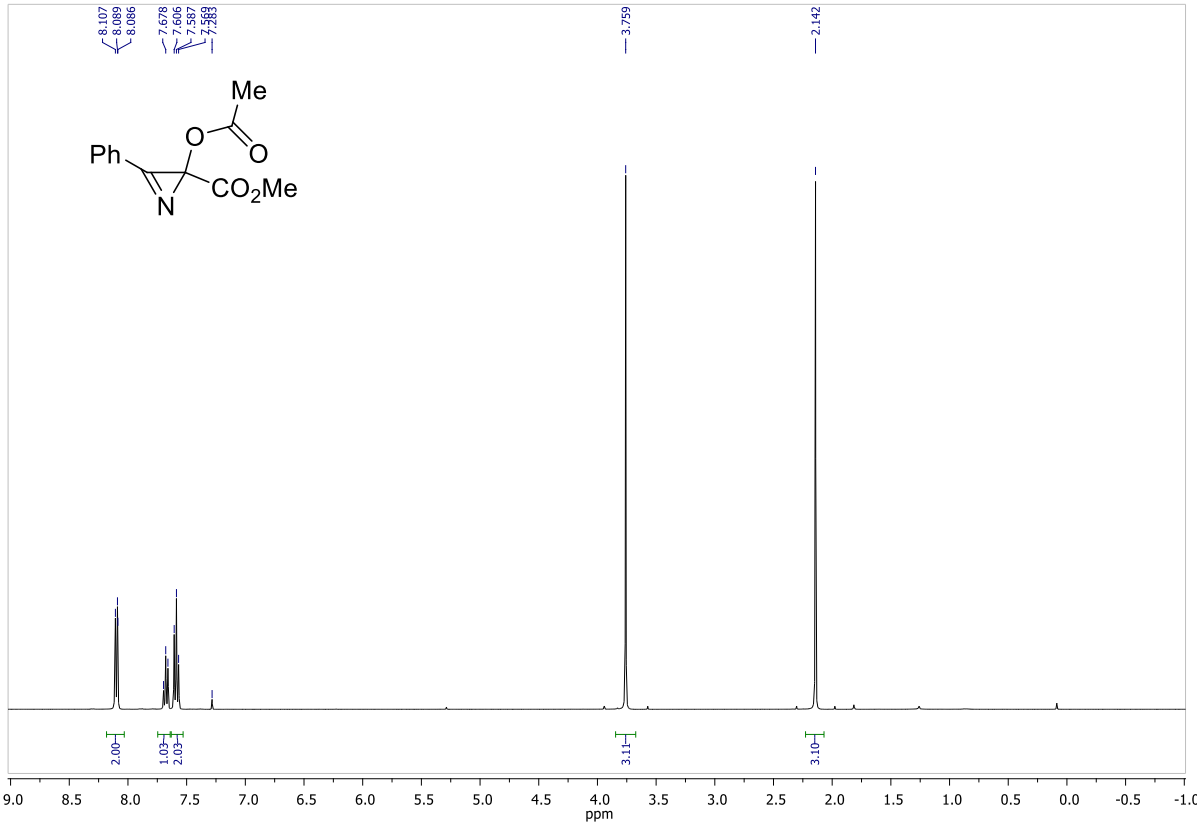
3. ^{1}H, ^{13}C NMR and 2D HMBC spectra

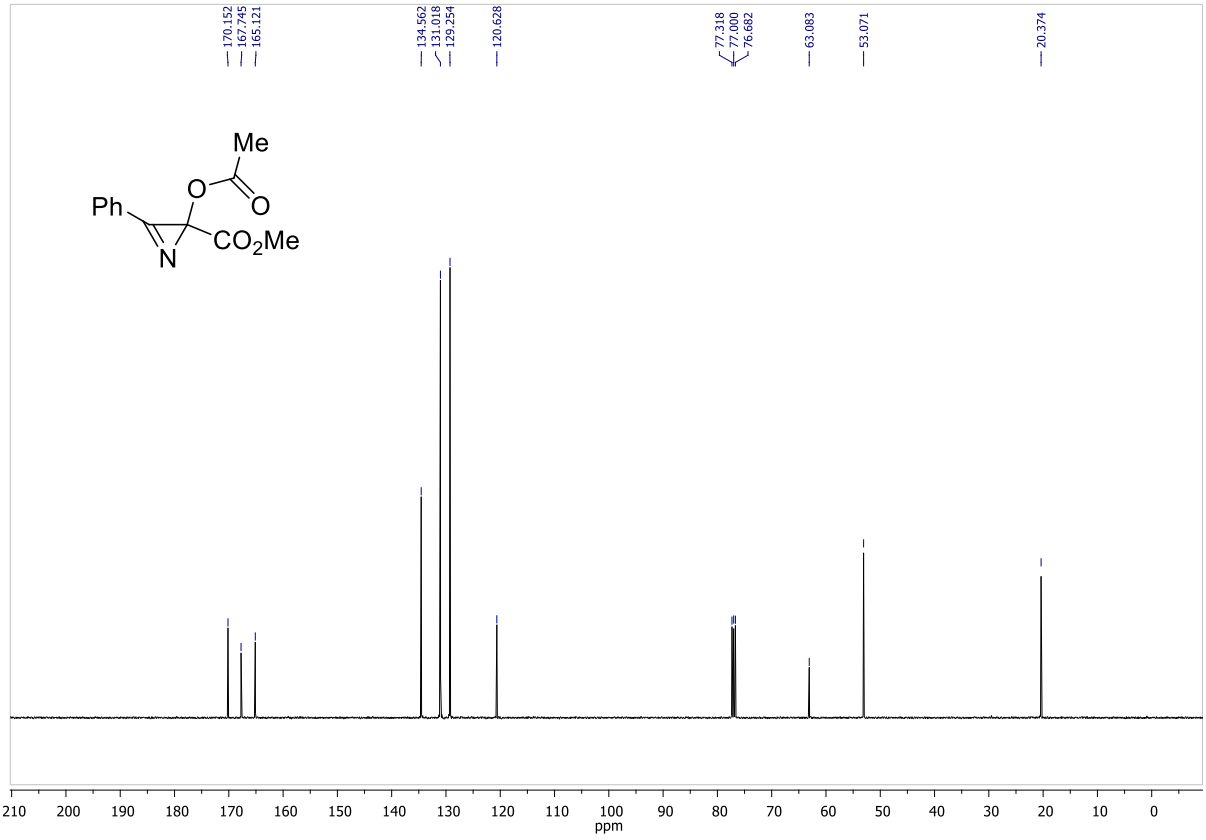
Methyl 3-phenyl-2-(thiophene-2-carbonyloxy)-2*H*-azirine-2-carboxylate (**2a**)



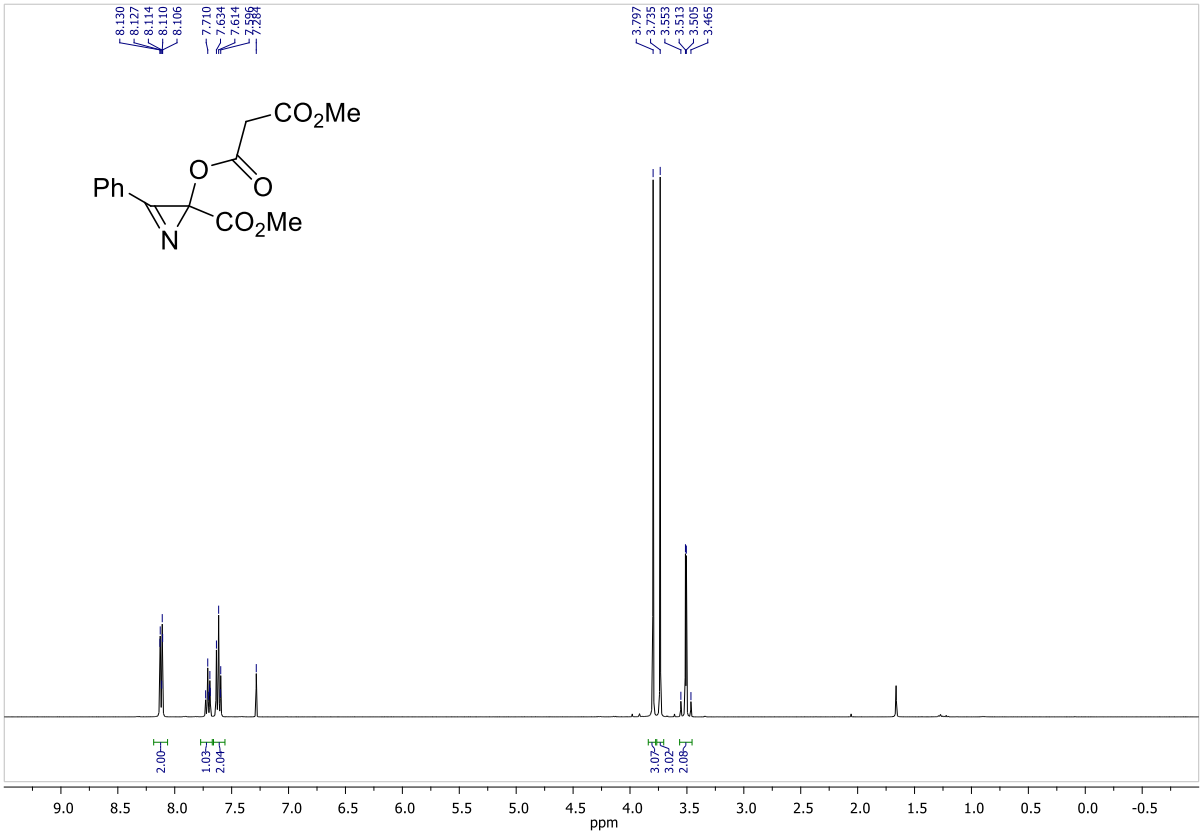


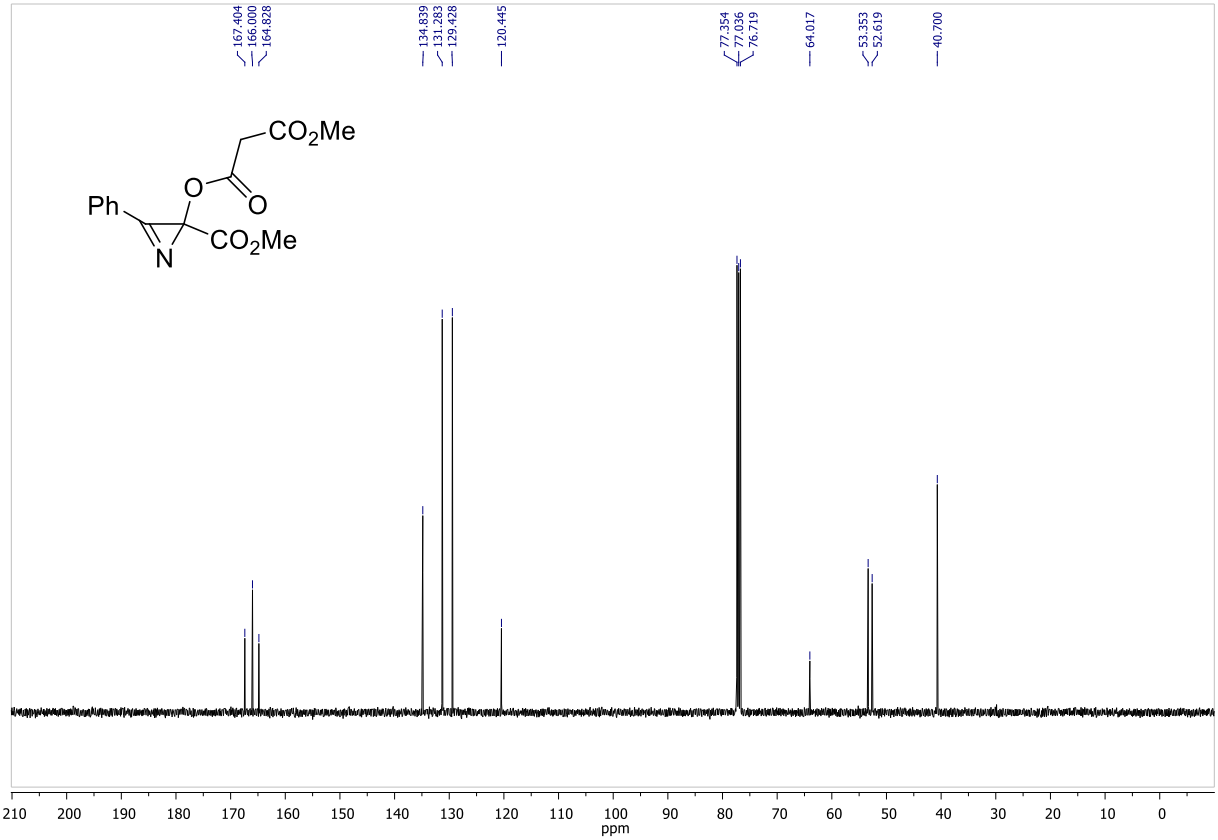
Methyl 2-acetoxy-3-phenyl-2*H*-azirine-2-carboxylate (**2b**)

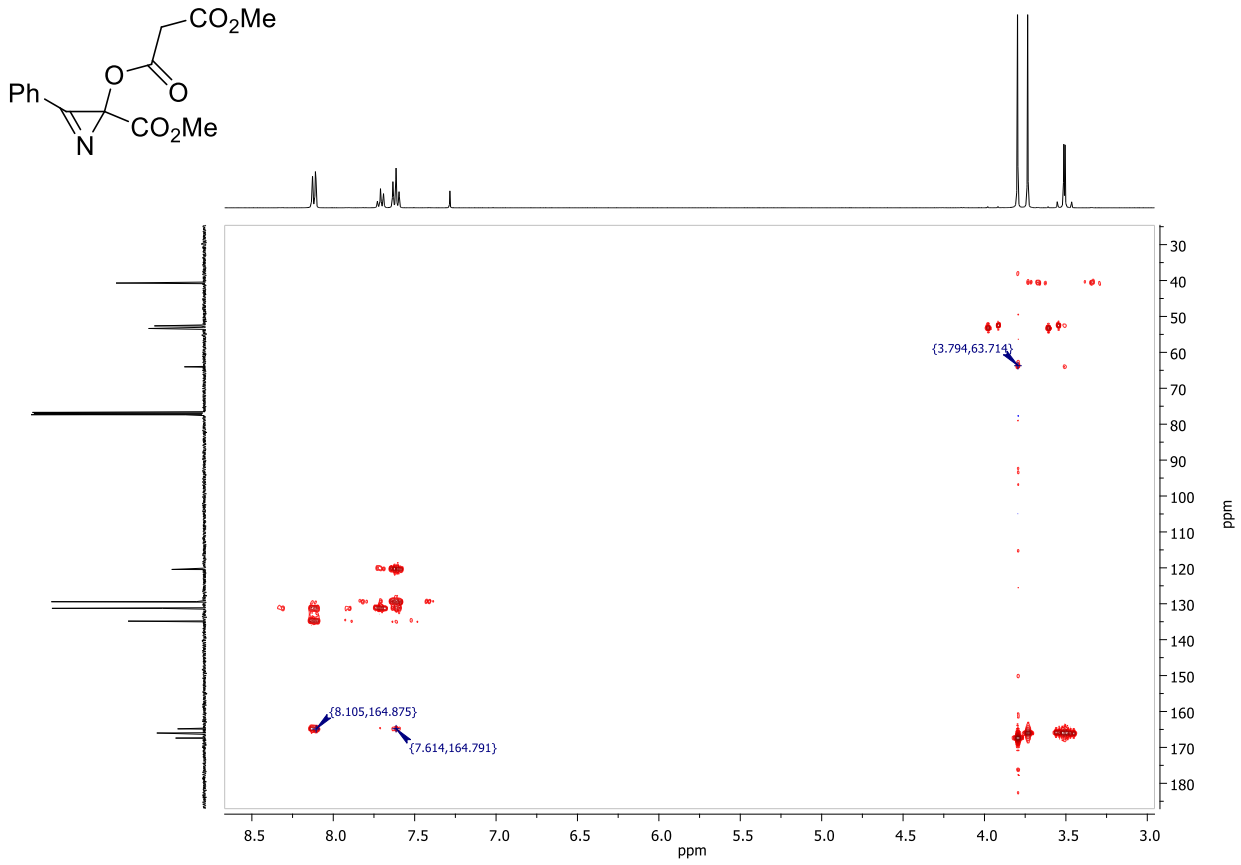




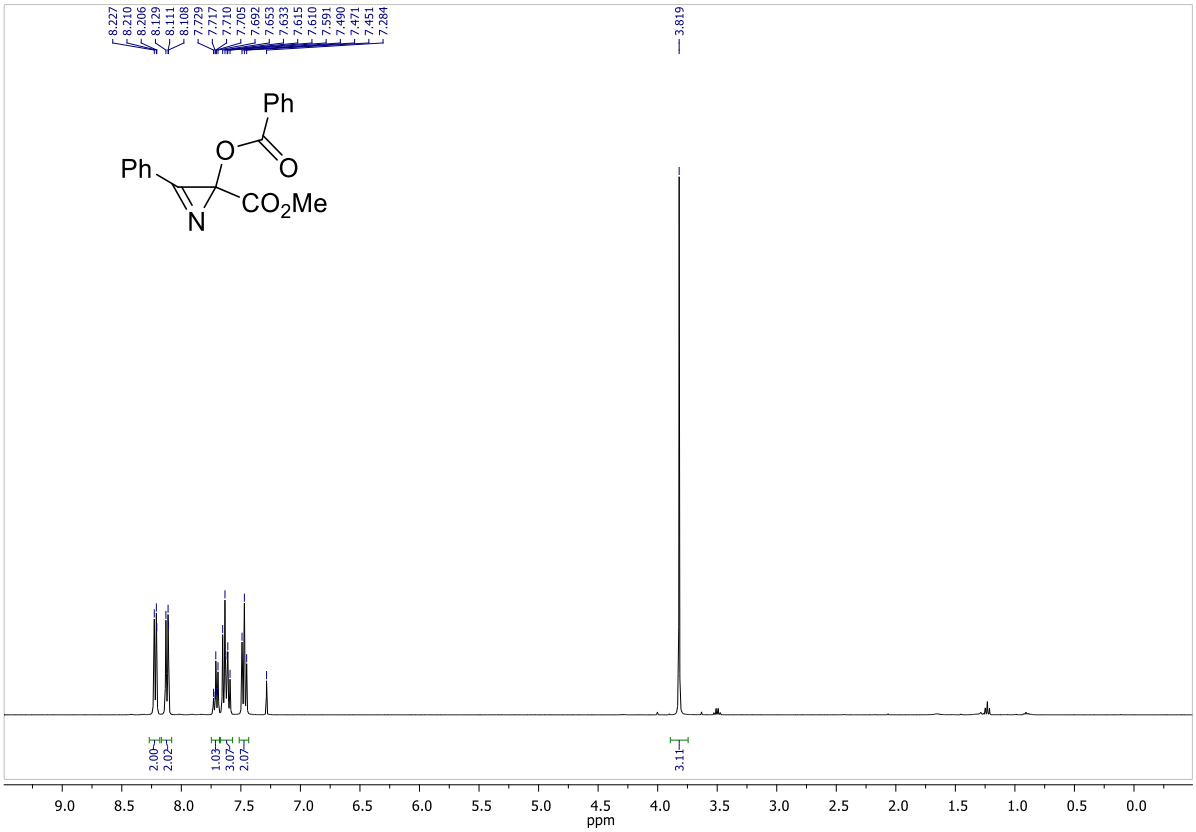
2-(Methoxycarbonyl)-3-phenyl-2*H*-azirin-2-yl methyl malonate (**2c**)

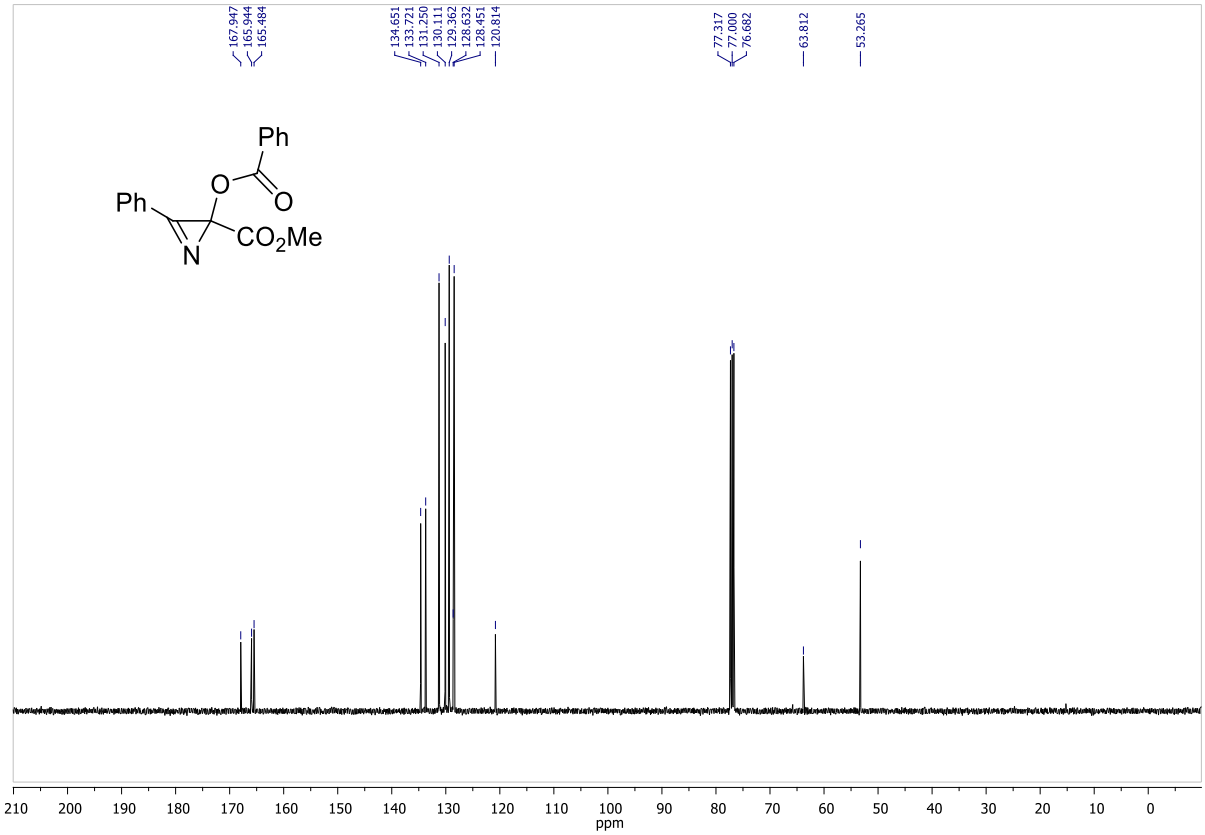




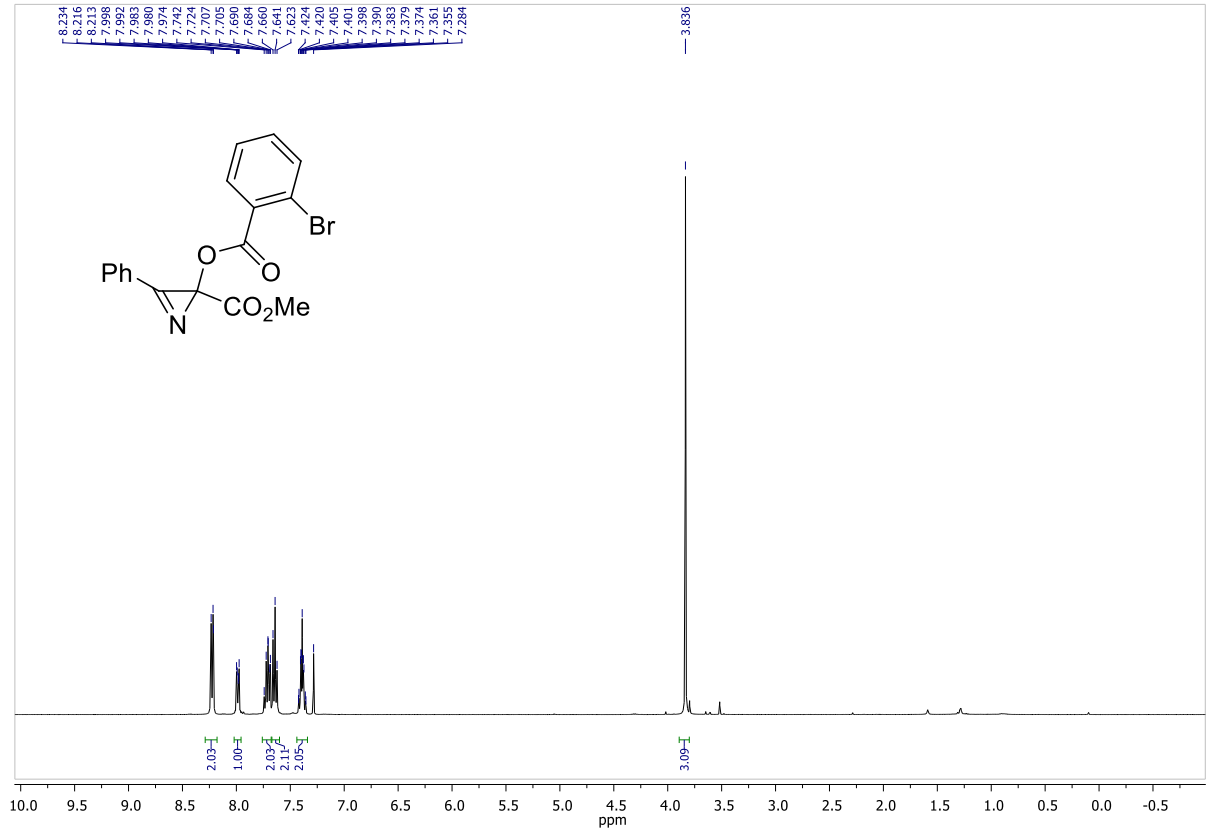

CO2Me
O
O
Ph
CO2Me
N
{3.794,63.714}
{8.105,164.875}
{7.614,164.791}
ppm
ppm

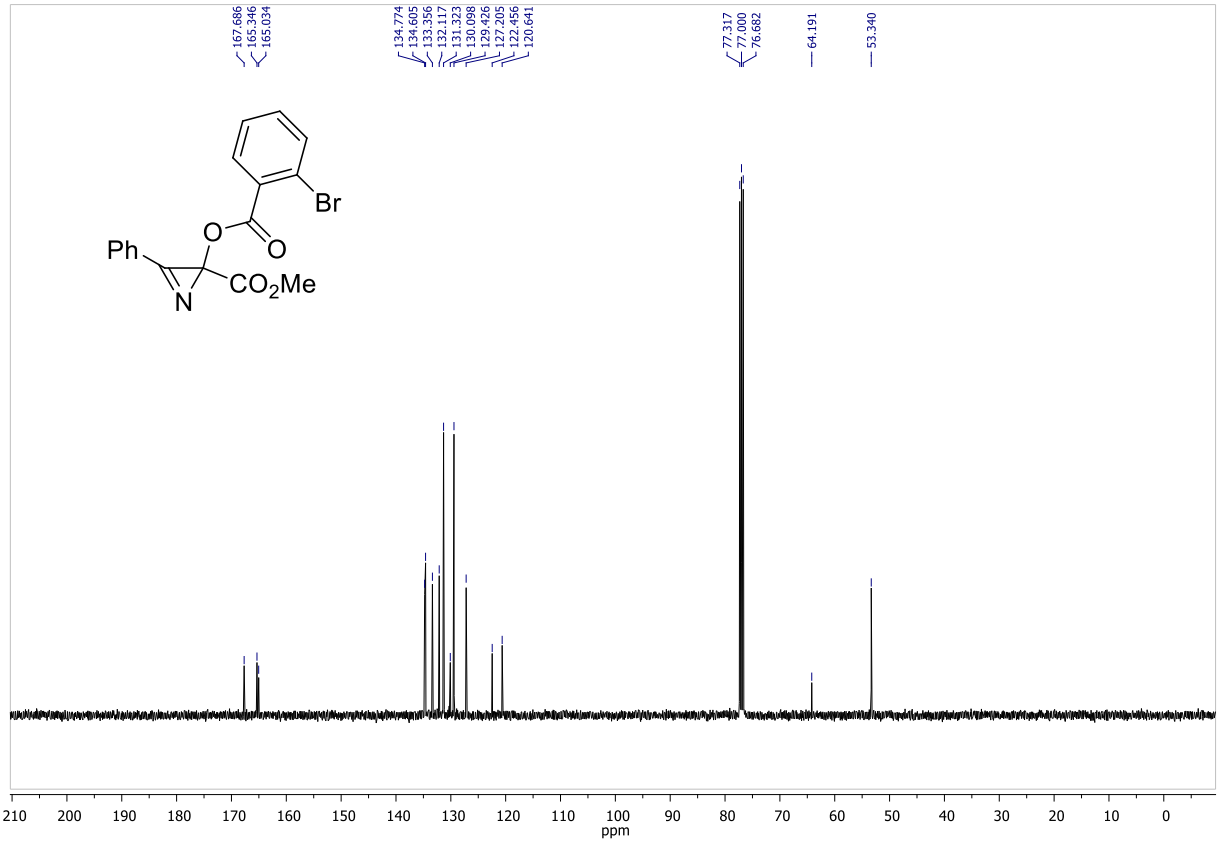
Methyl 2-(benzoyloxy)-3-phenyl-2*H*-azirine-2-carboxylate (**2d**)



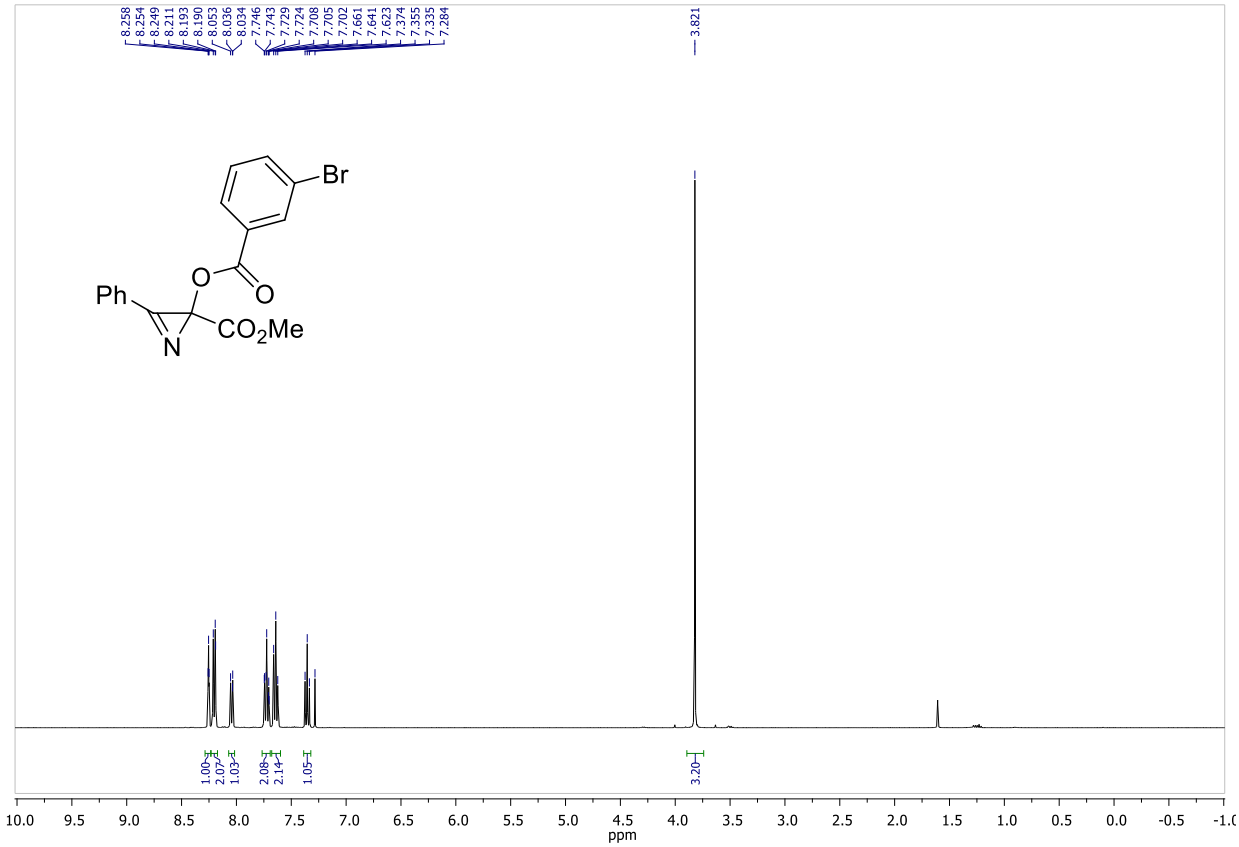


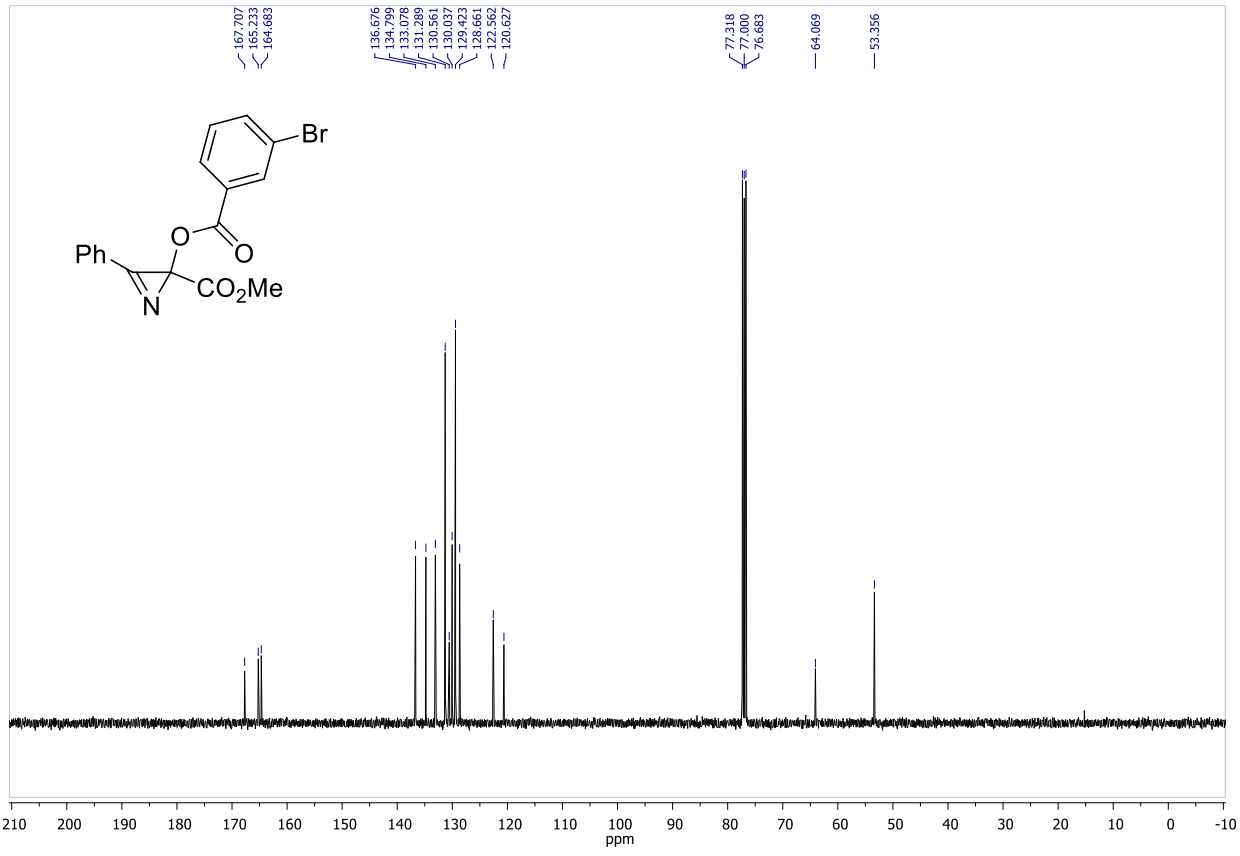
Methyl 2-(2-bromobenzoyloxy)-3-phenyl-2*H*-azirine-2-carboxylate (**2e**)



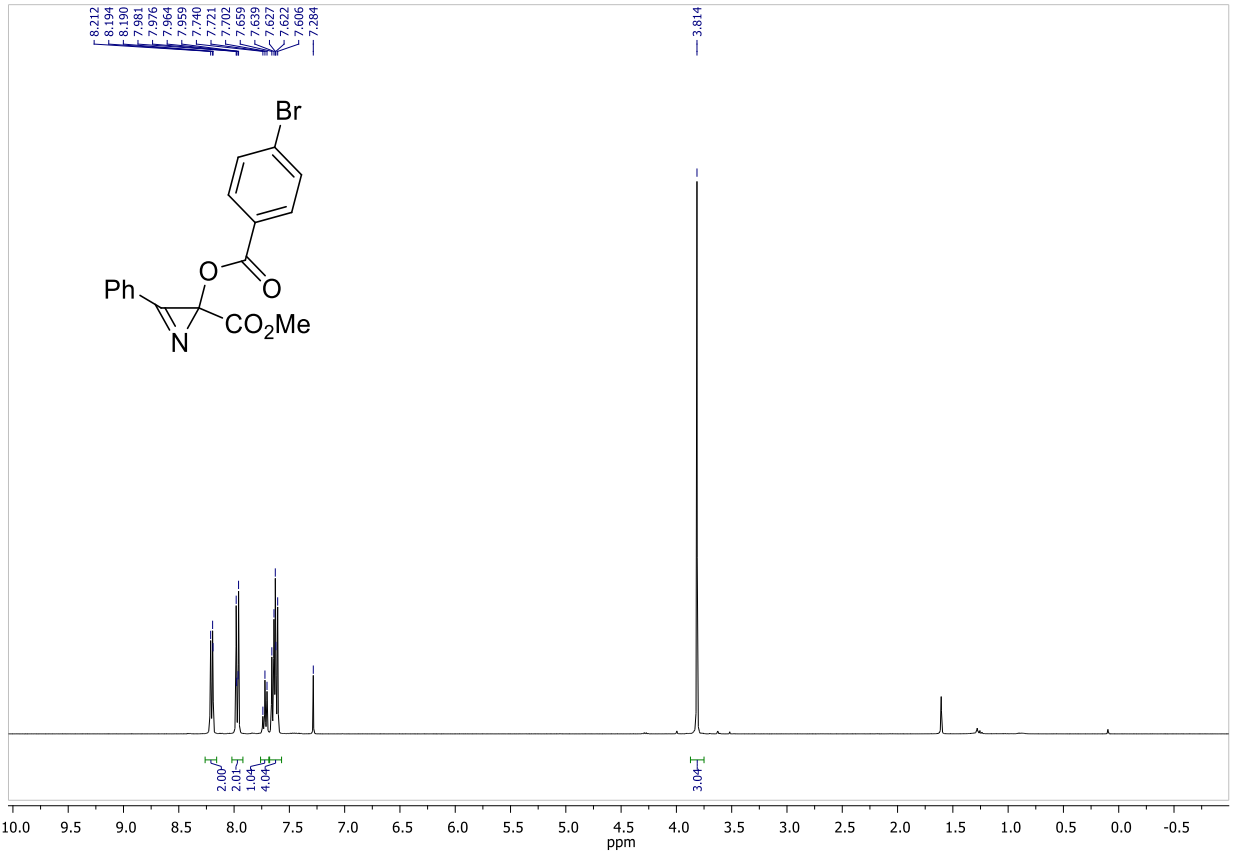


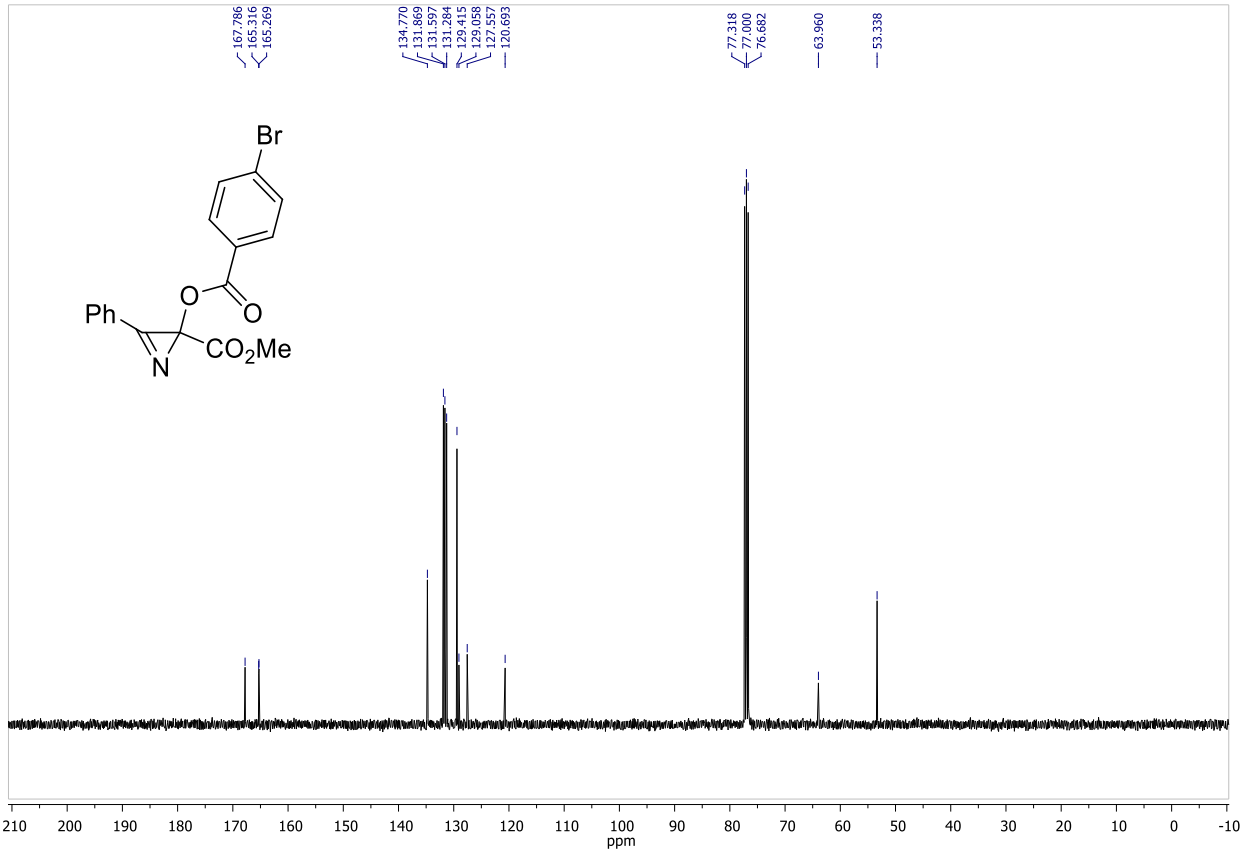
Methyl 2-(3-bromobenzoyloxy)-3-phenyl-2*H*-azirine-2-carboxylate (**2f**)



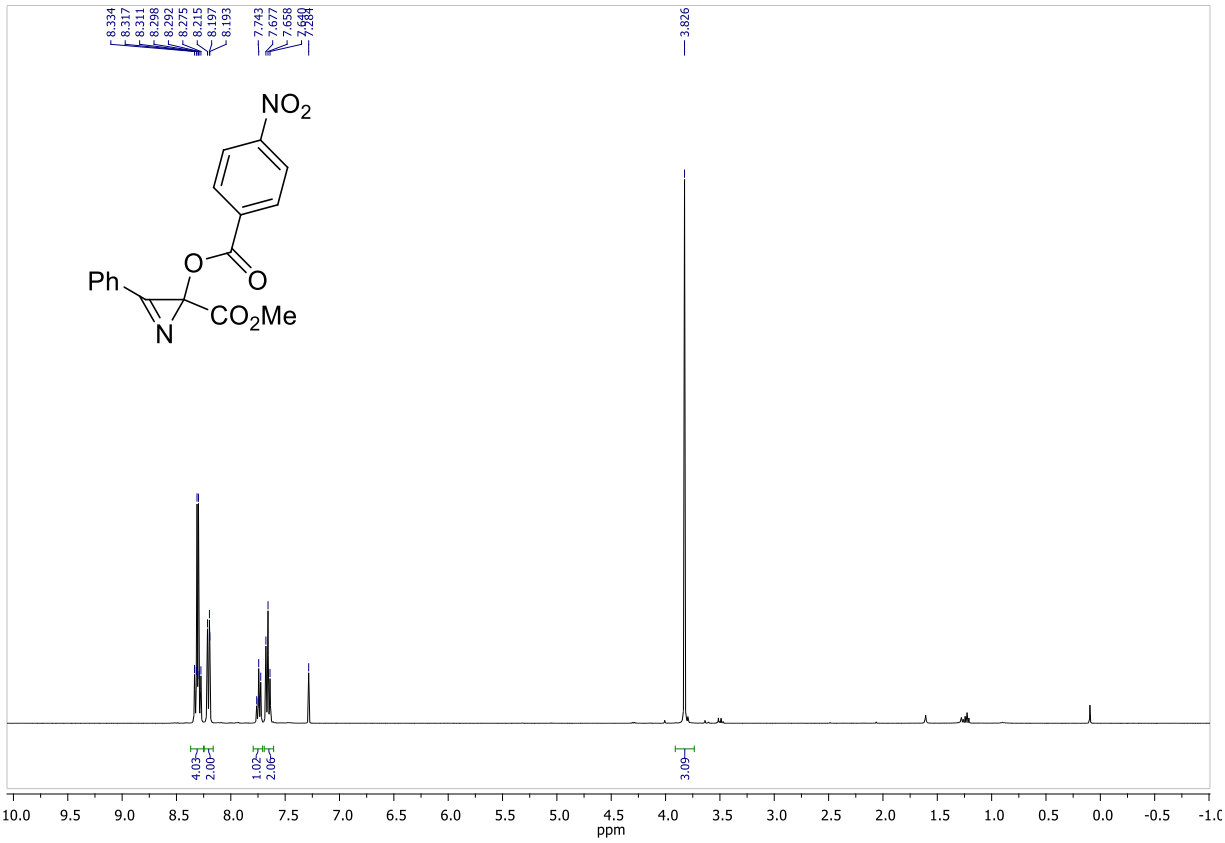


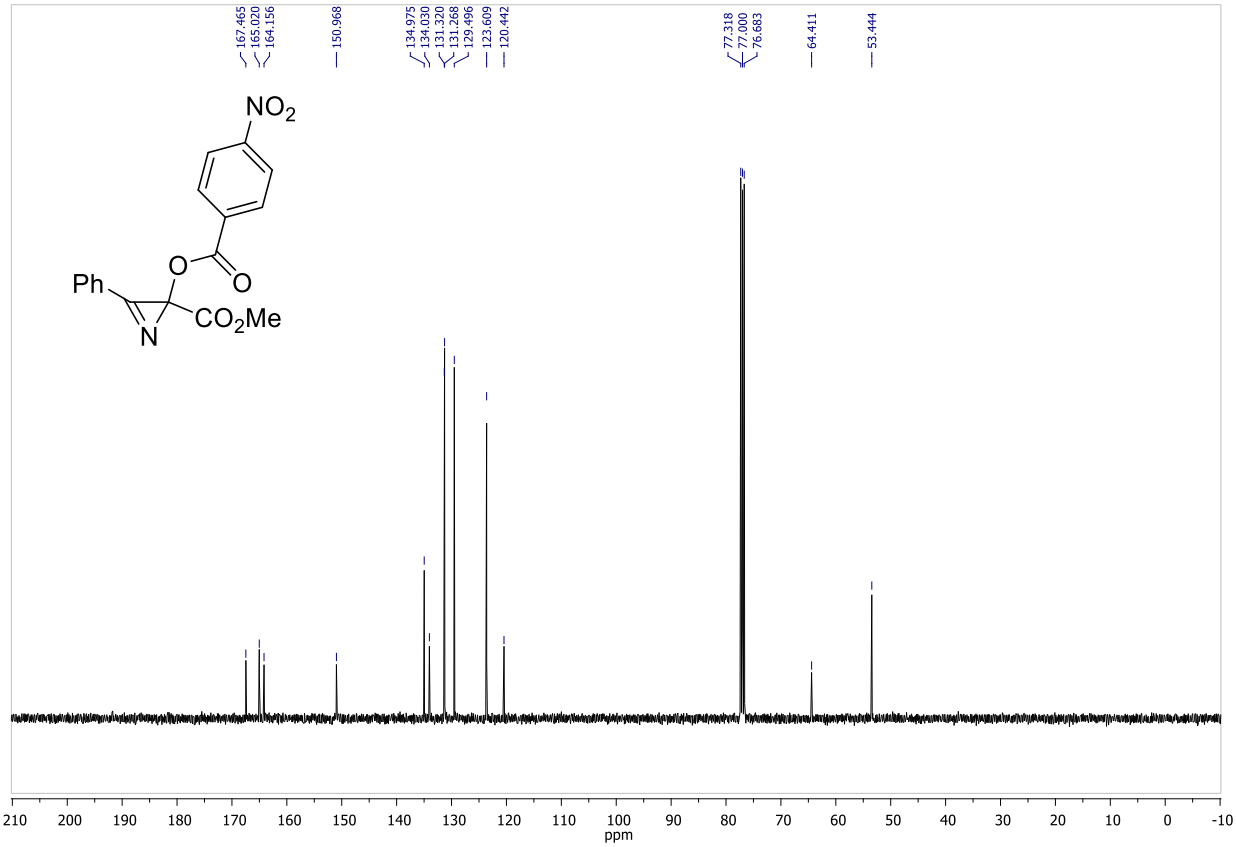
Methyl 2-(4-bromobenzoyloxy)-3-phenyl-2*H*-azirine-2-carboxylate (**2g**)



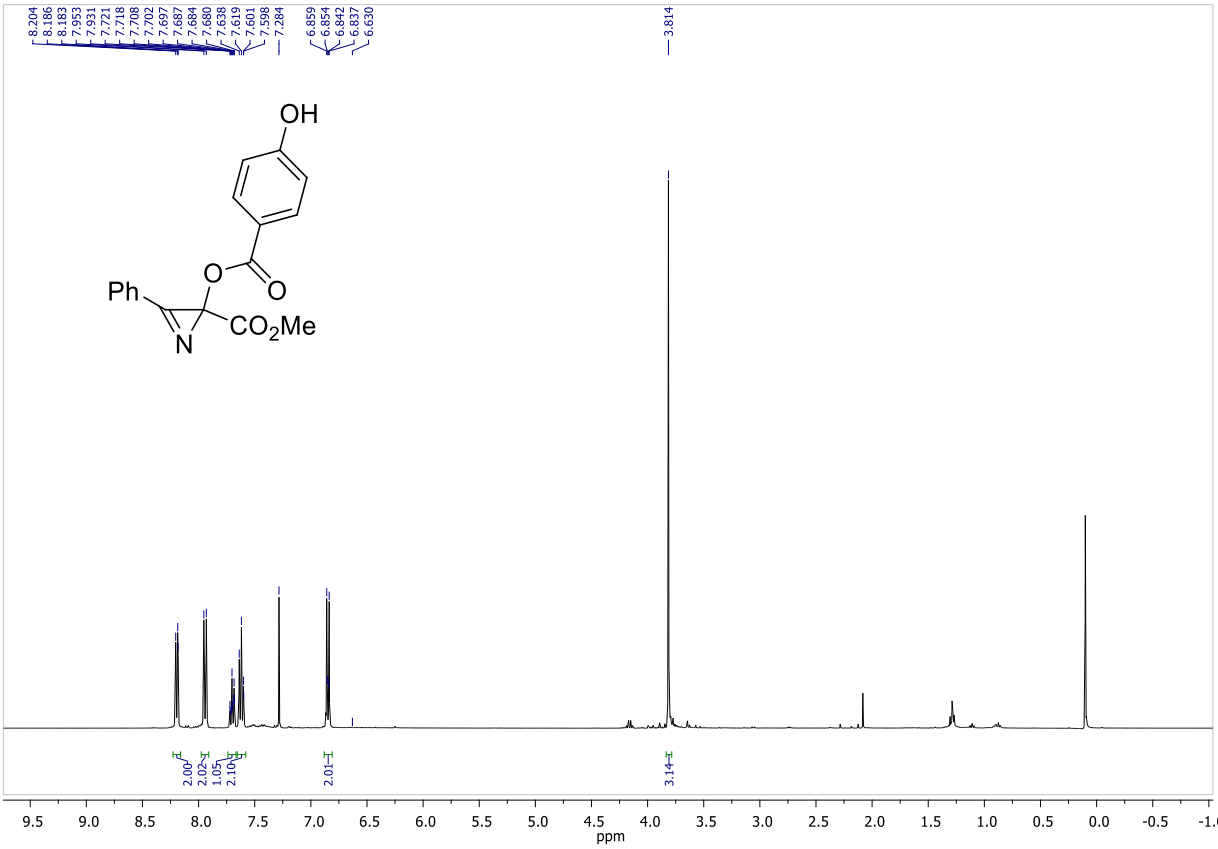


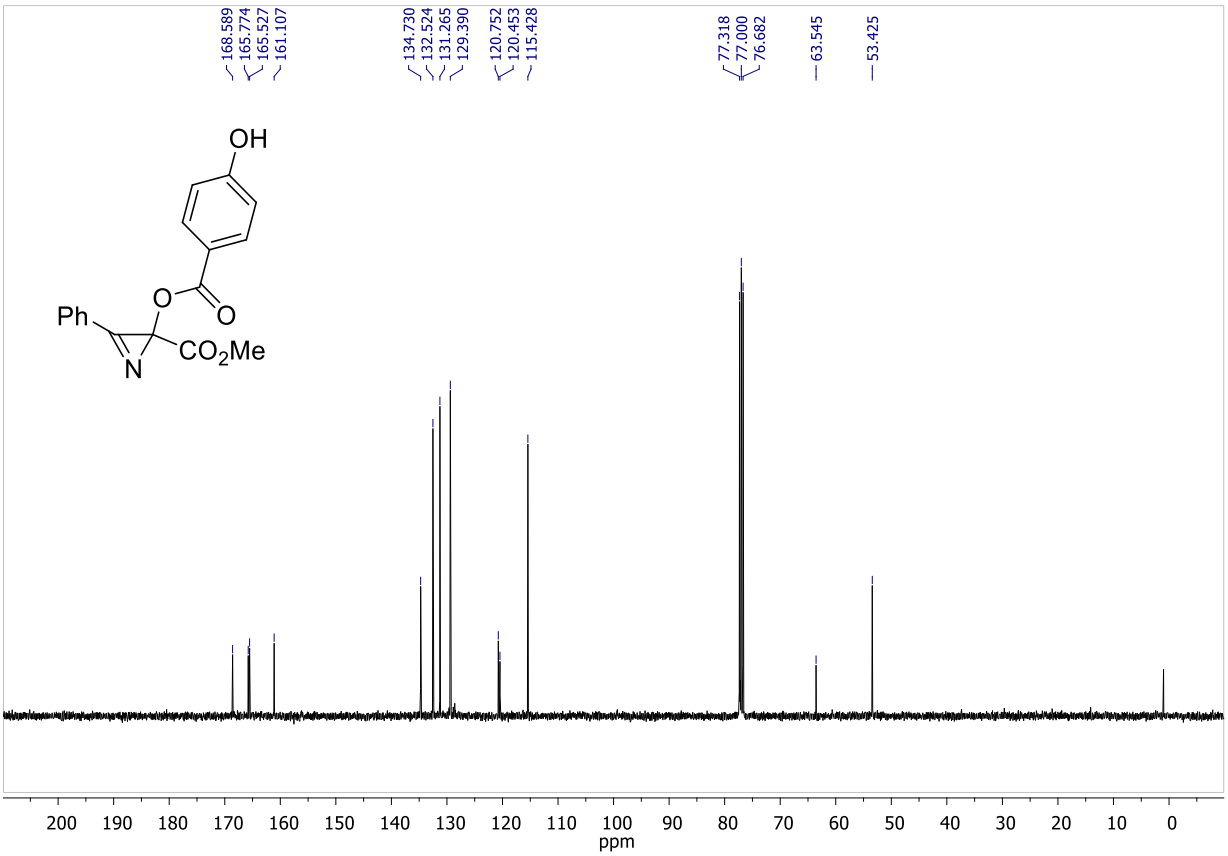
Methyl 2-(4-nitrobenzoyloxy)-3-phenyl-2*H*-azirine-2-carboxylate (**2h**)



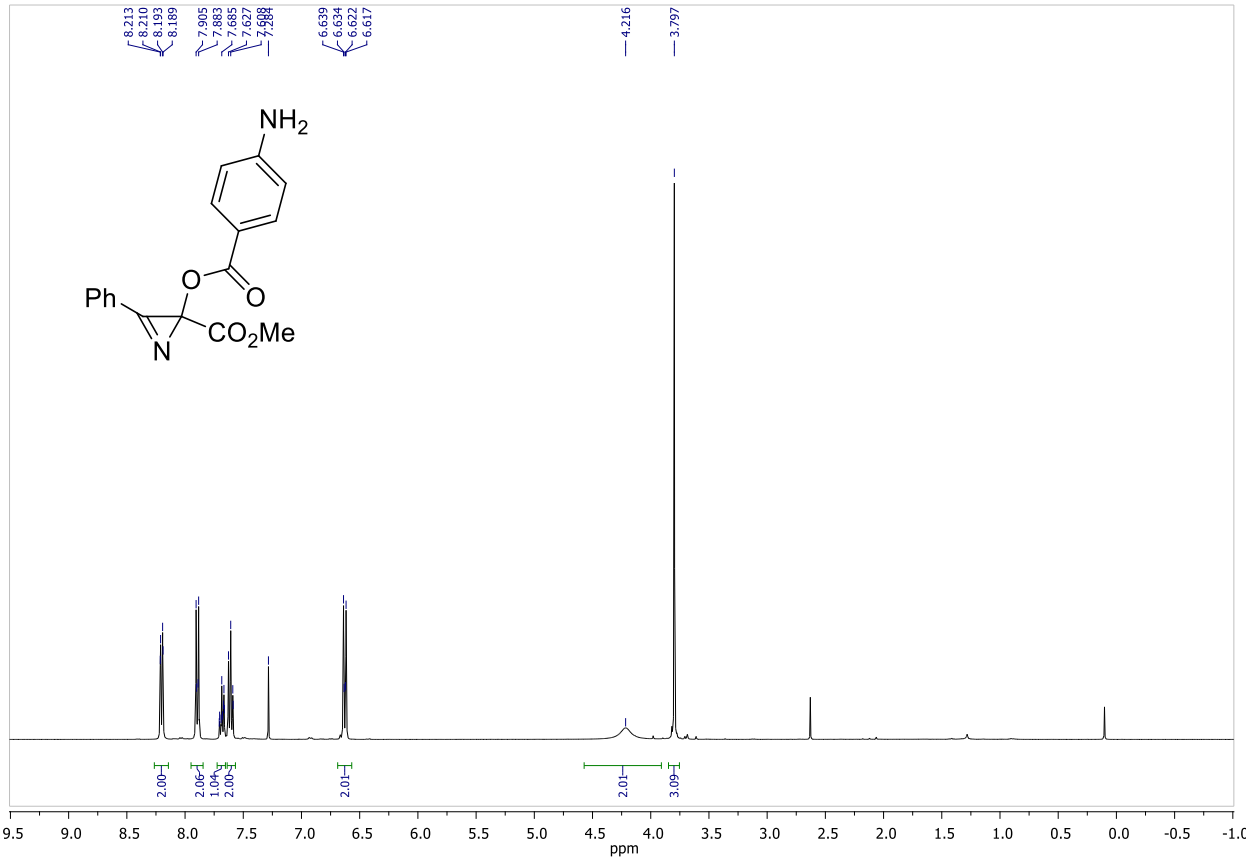


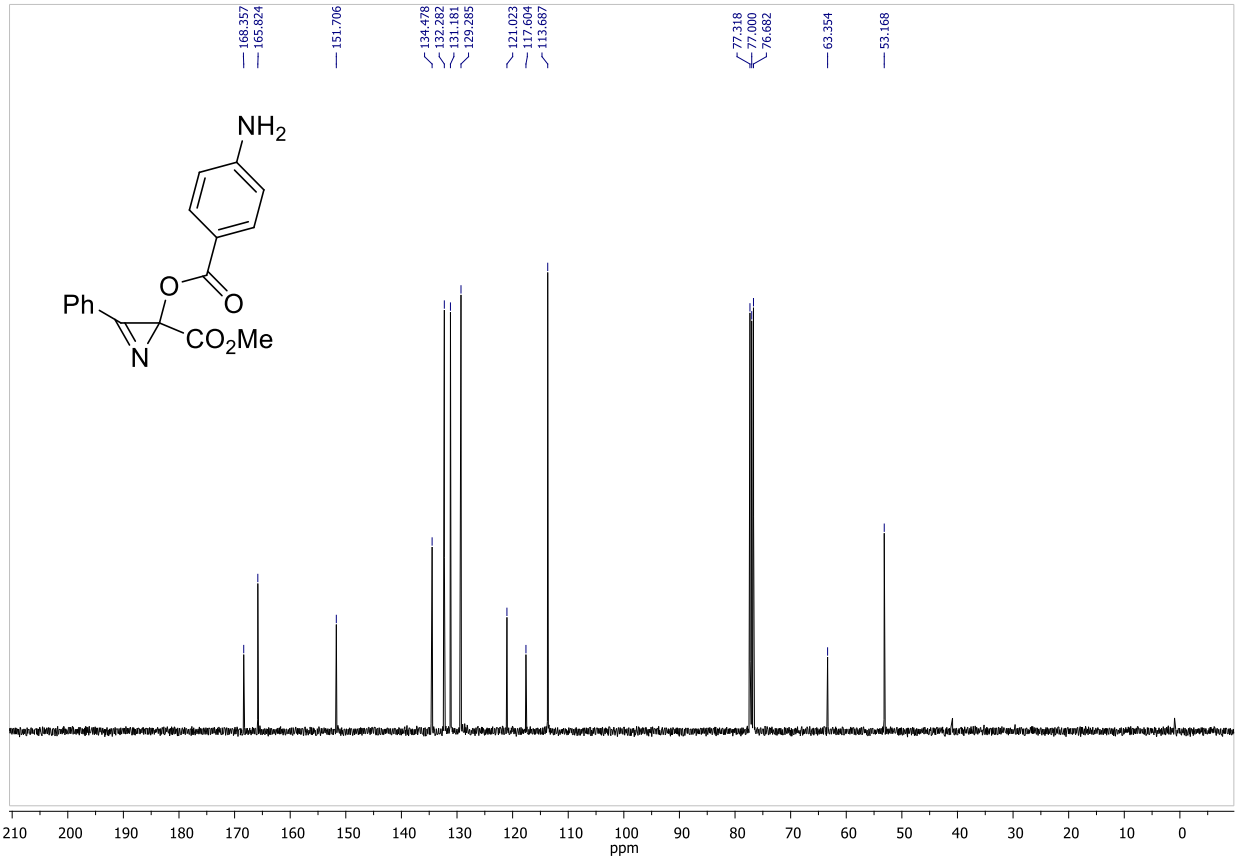
Methyl 2-(4-hydroxybenzoyloxy)-3-phenyl-2*H*-azirine-2-carboxylate (**2i**)



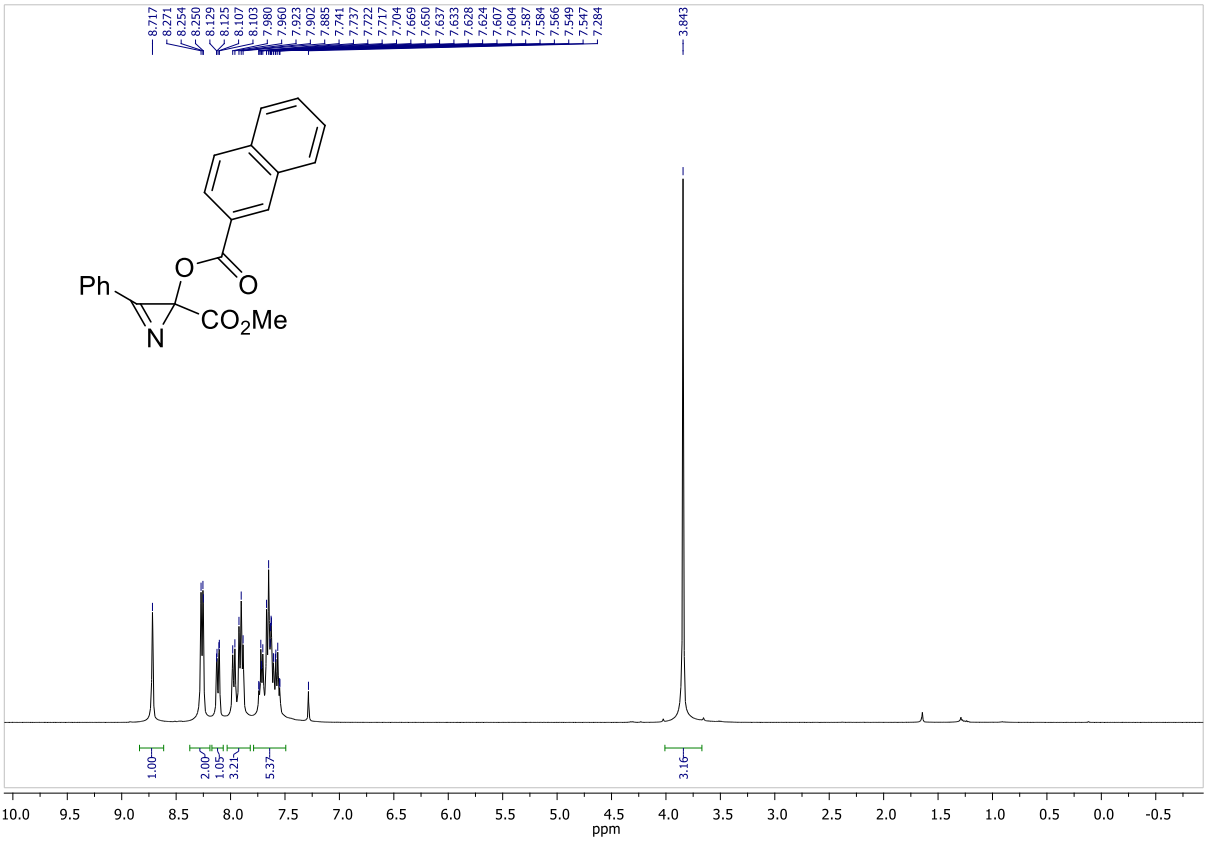


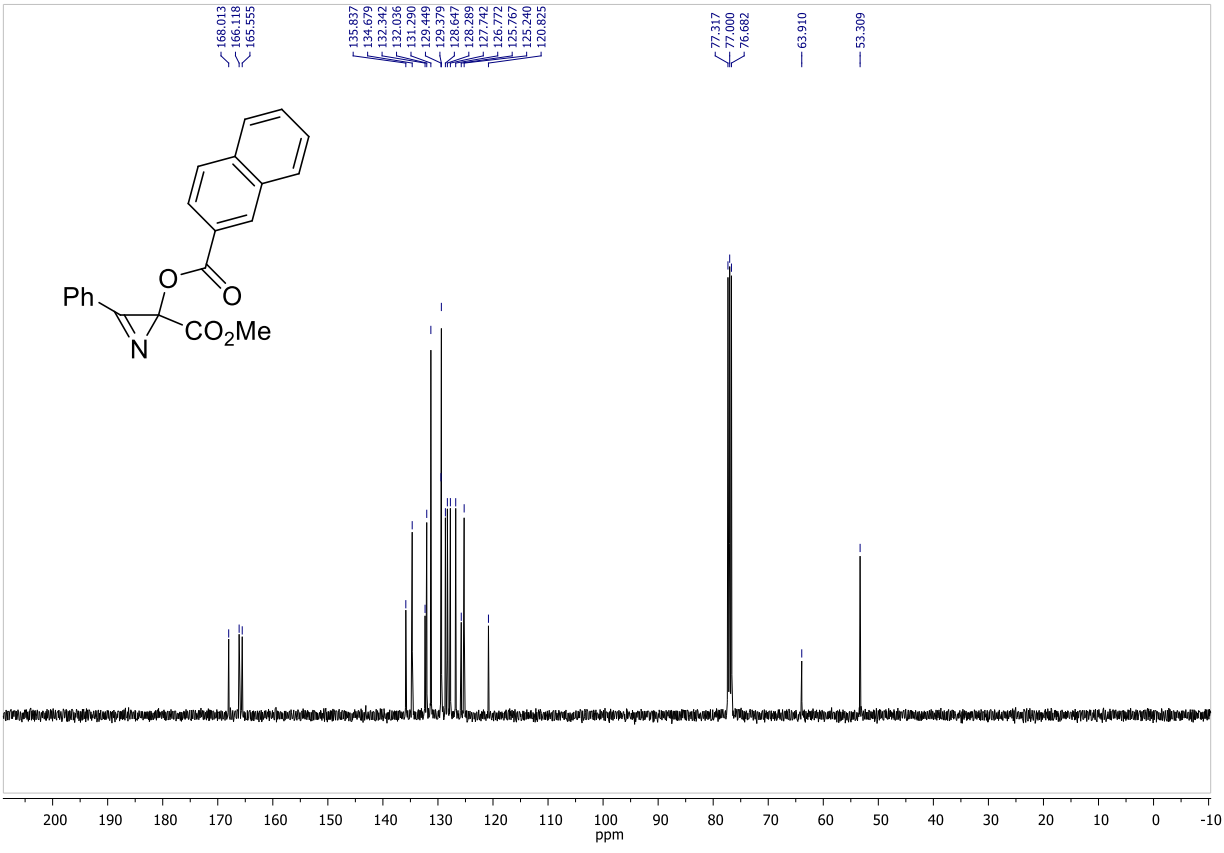
Methyl 2-(4-aminobenzoyloxy)-3-phenyl-2*H*-azirine-2-carboxylate (**2j**)



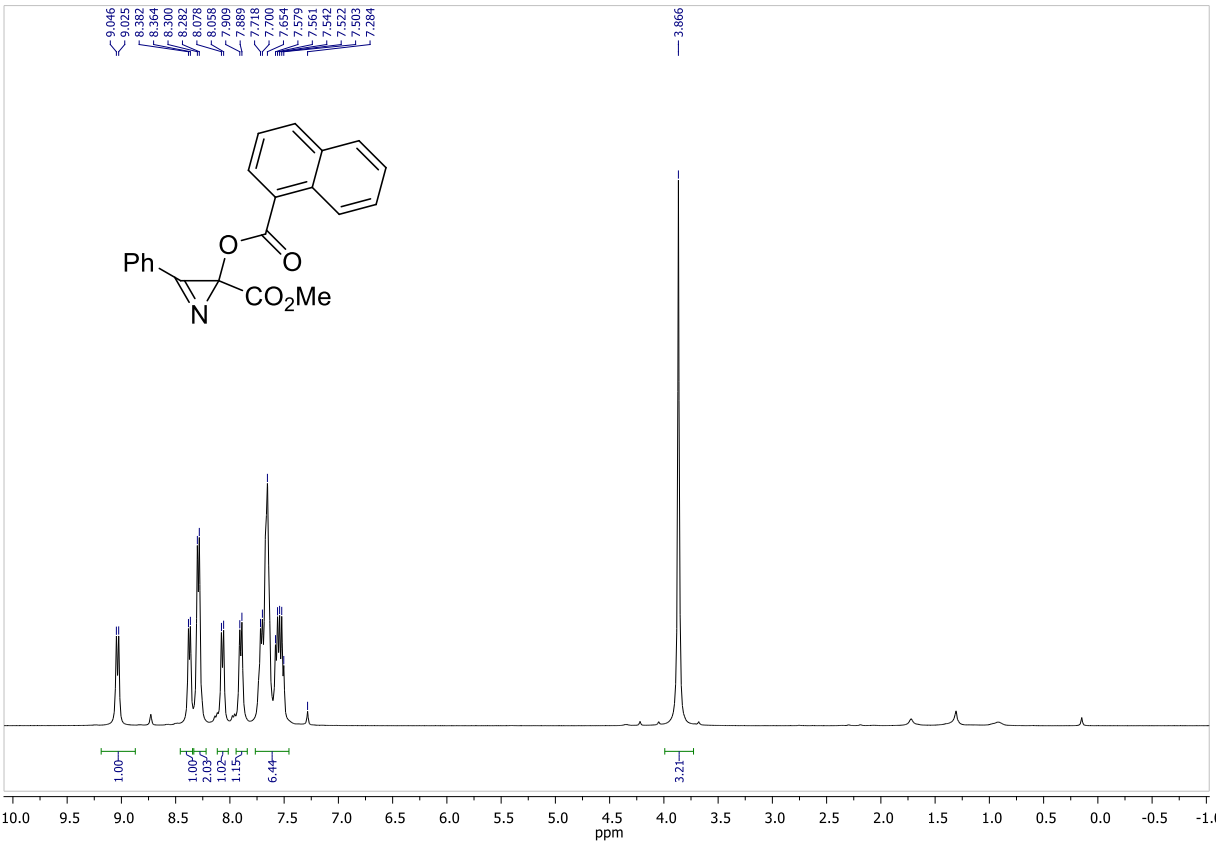


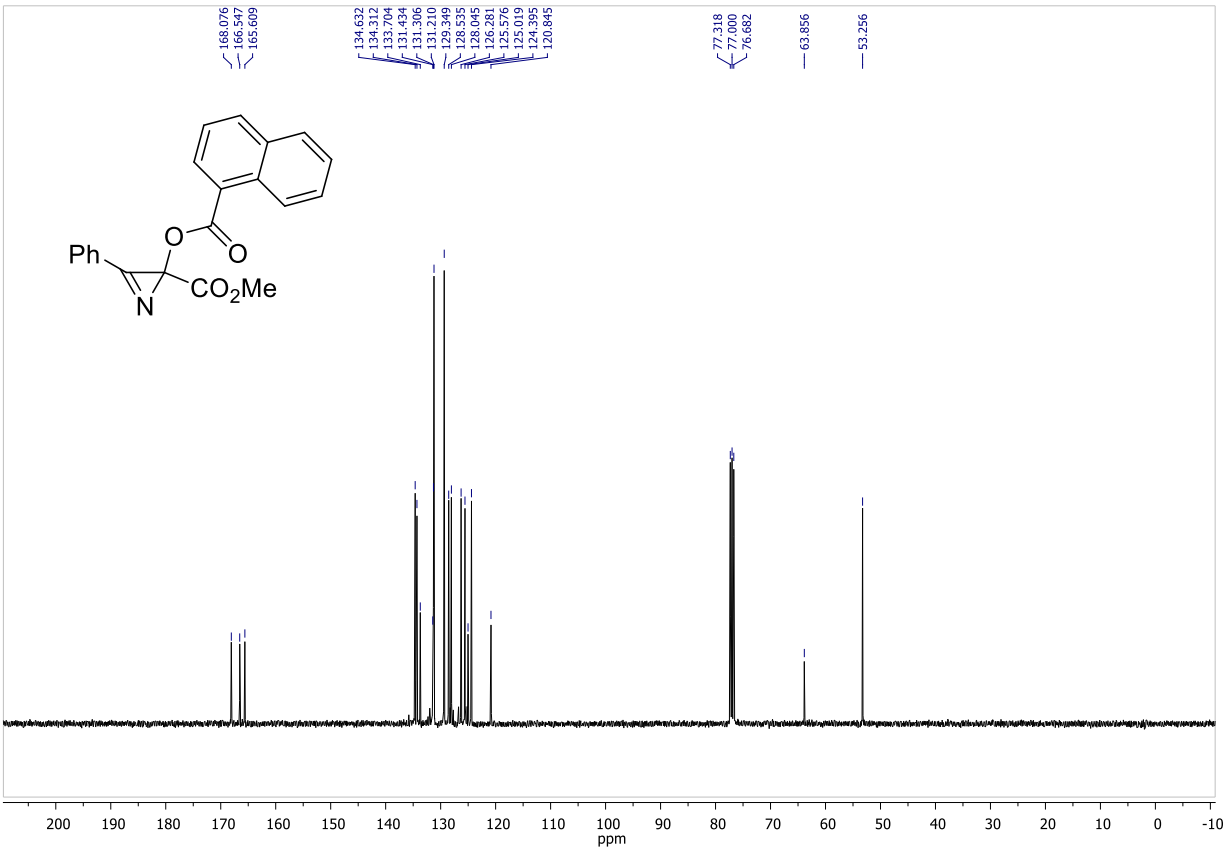
Methyl 2-(2-naphthoyloxy)-3-phenyl-2*H*-azirine-2-carboxylate (**2k**)



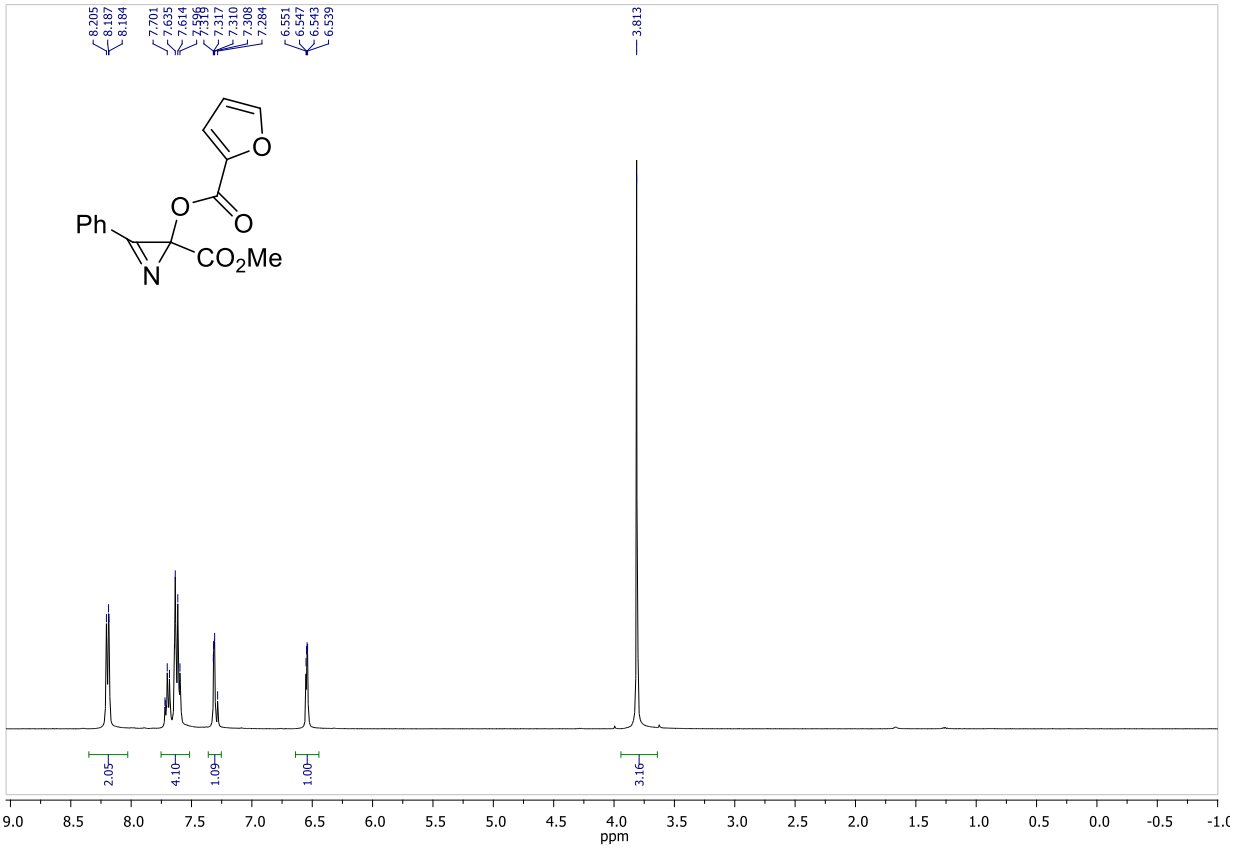


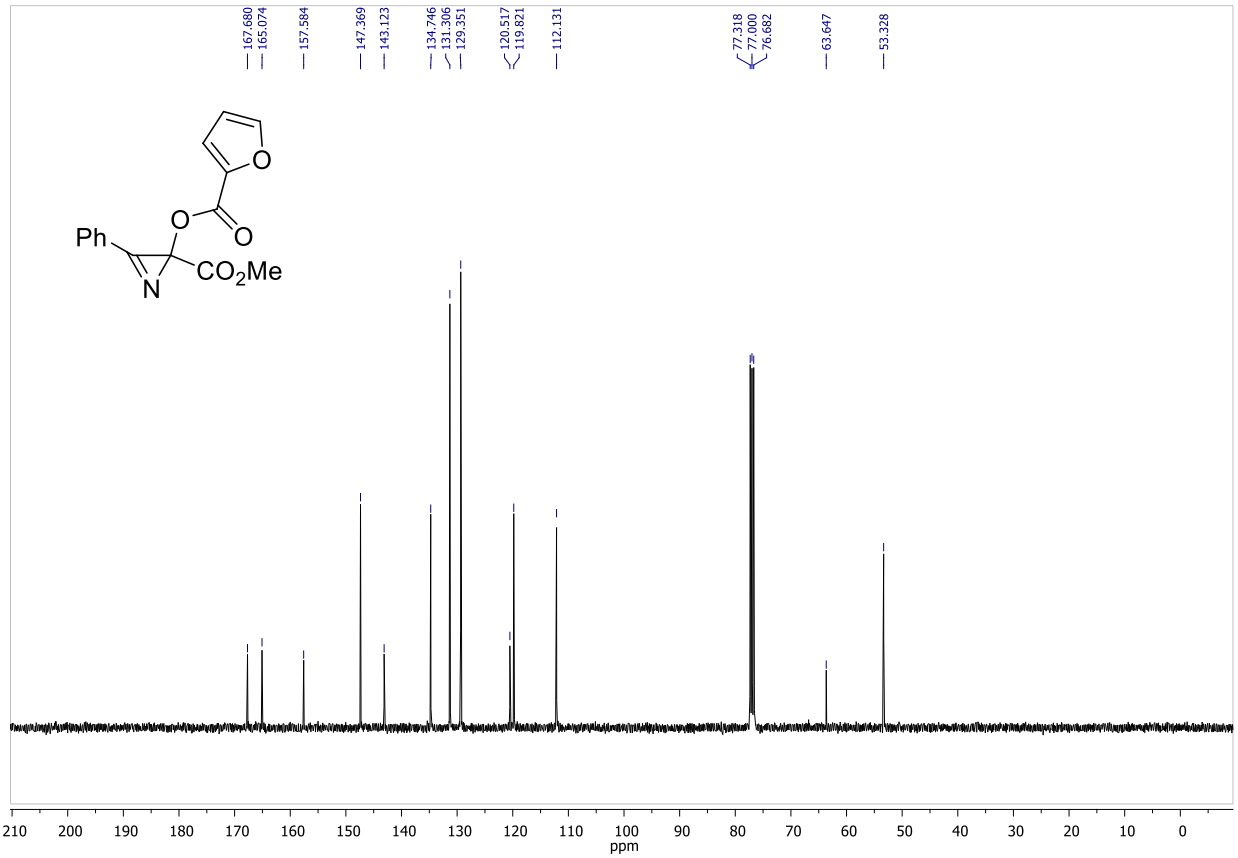
Methyl 2-((1-naphthoyl)oxy)-3-phenyl-2*H*-azirine-2-carboxylate (**2l**)



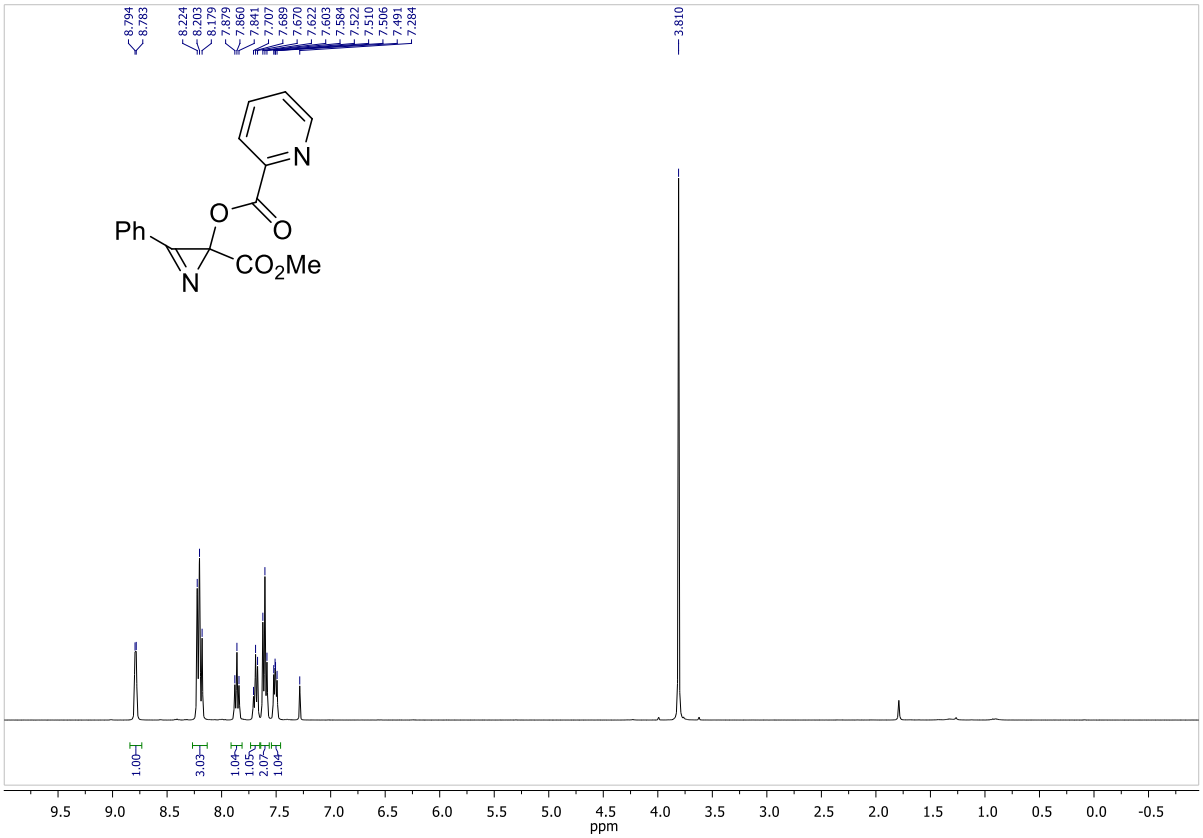


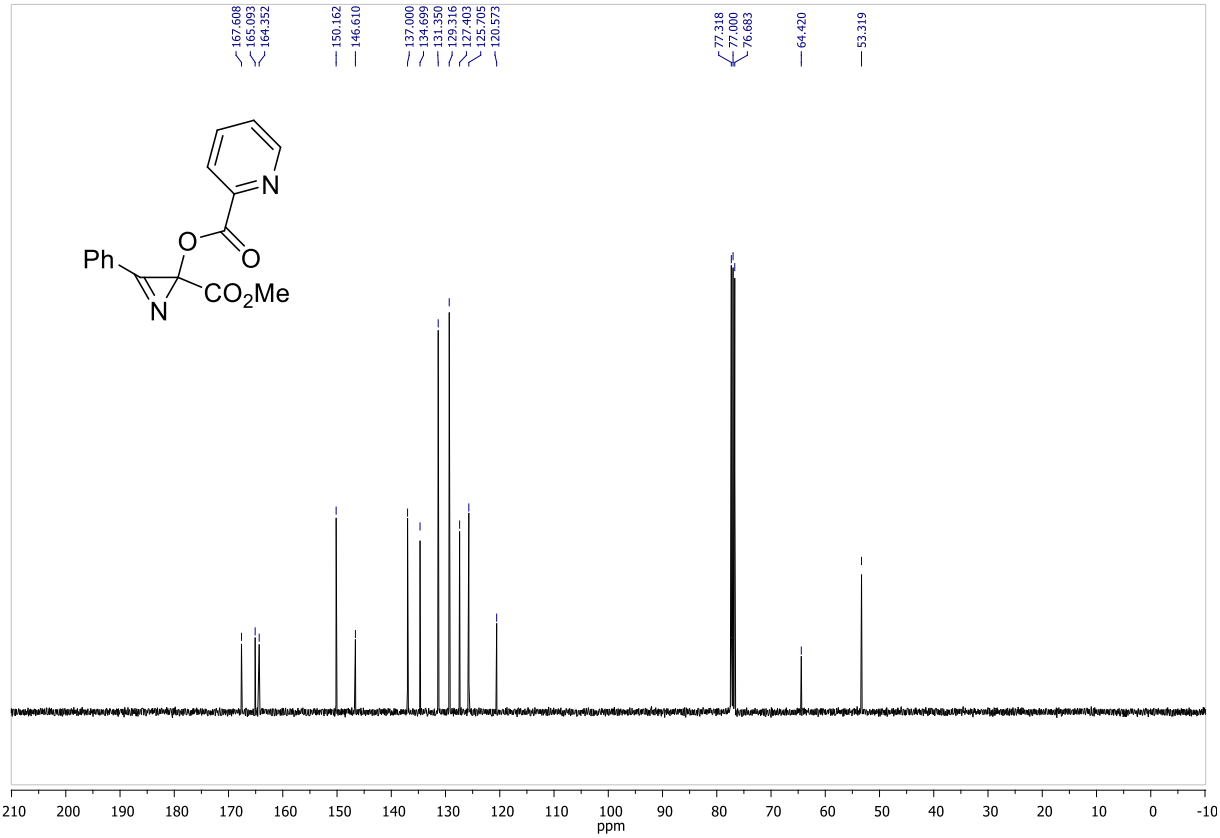
Methyl 2-(furan-2-carbonyloxy)-3-phenyl-2*H*-azirine-2-carboxylate (**2m**)



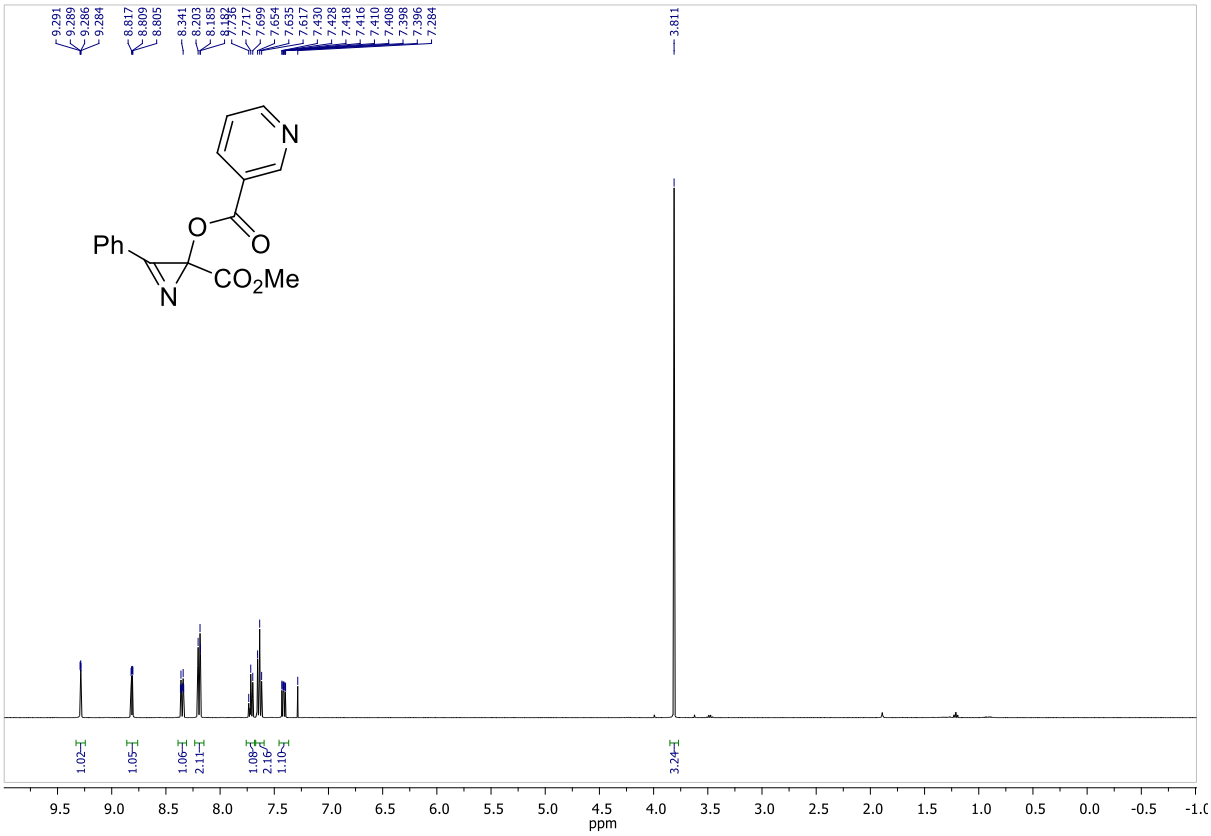


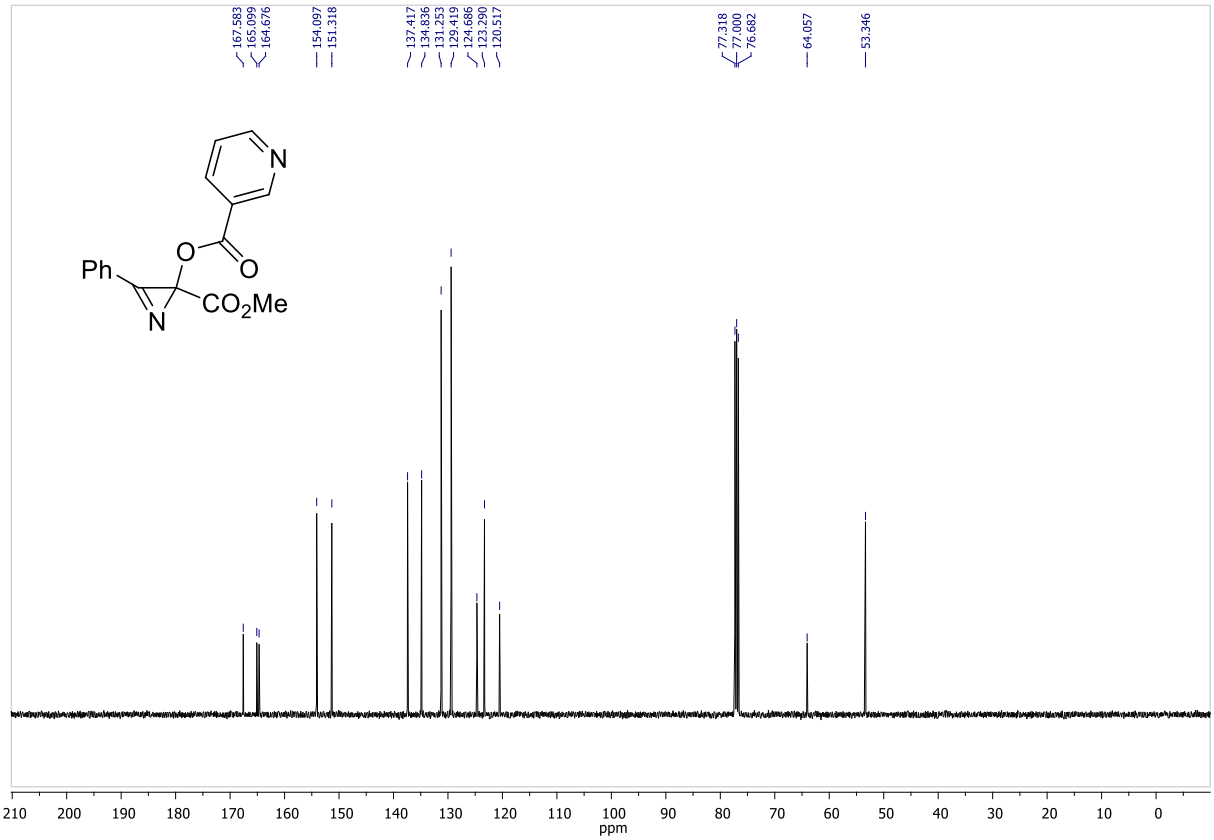
2-(Methoxycarbonyl)-3-phenyl-2*H*-azirin-2-yl picolinate (**2n**)



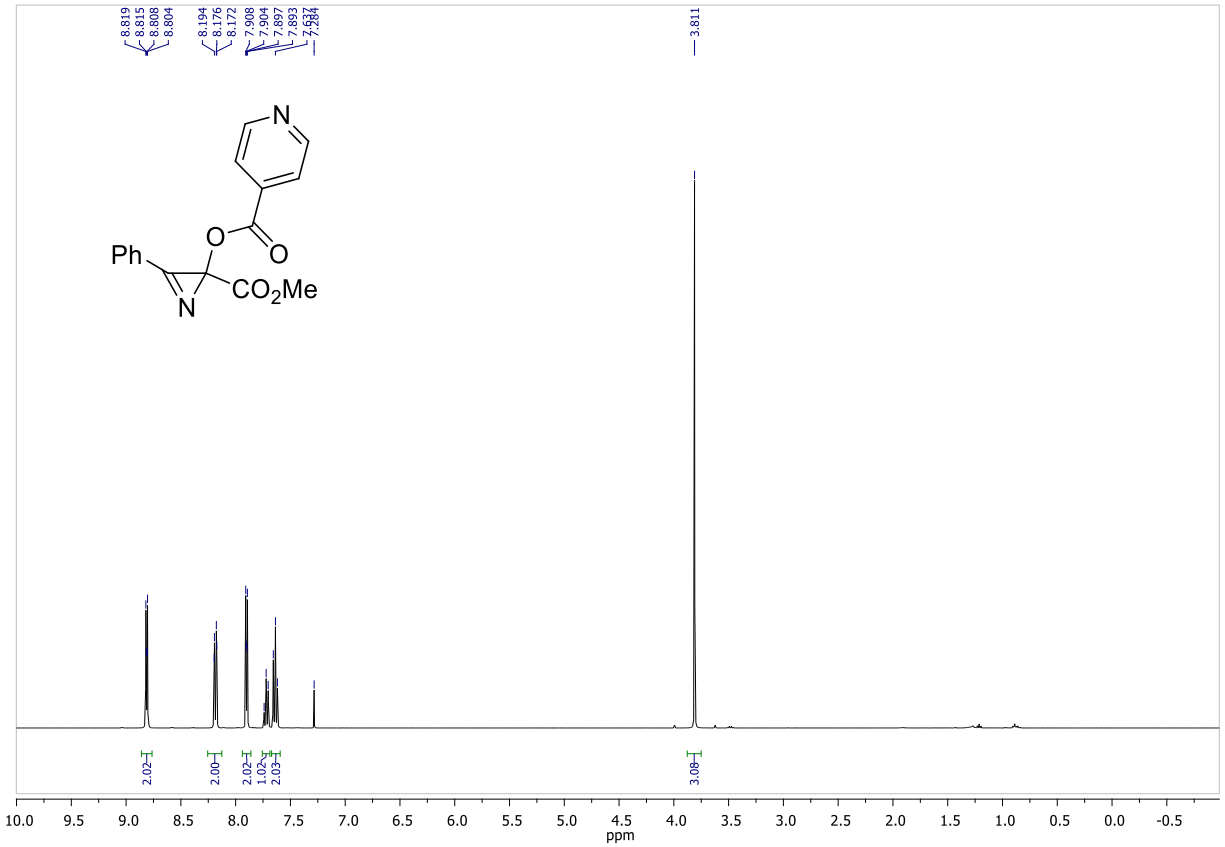


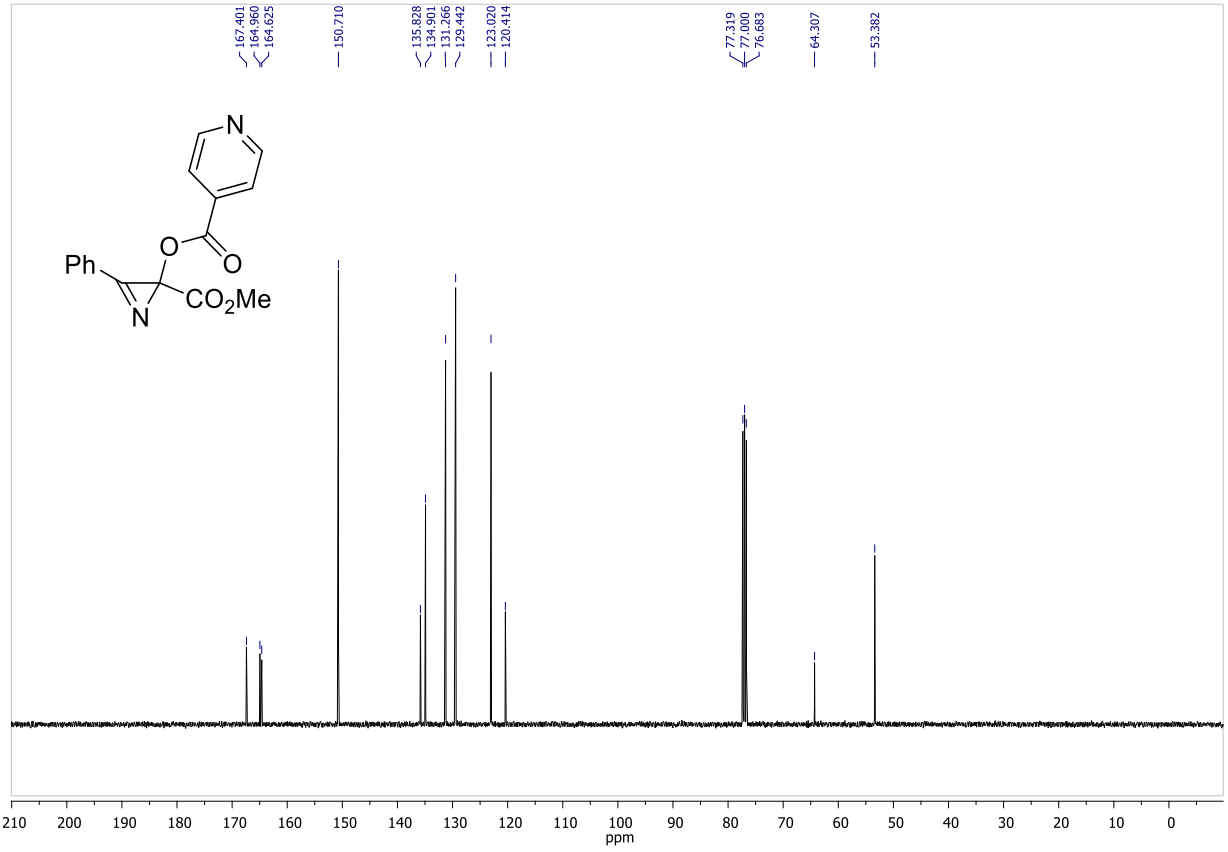
2-(Methoxycarbonyl)-3-phenyl-2*H*-azirin-2-yl nicotinate (**2o**)



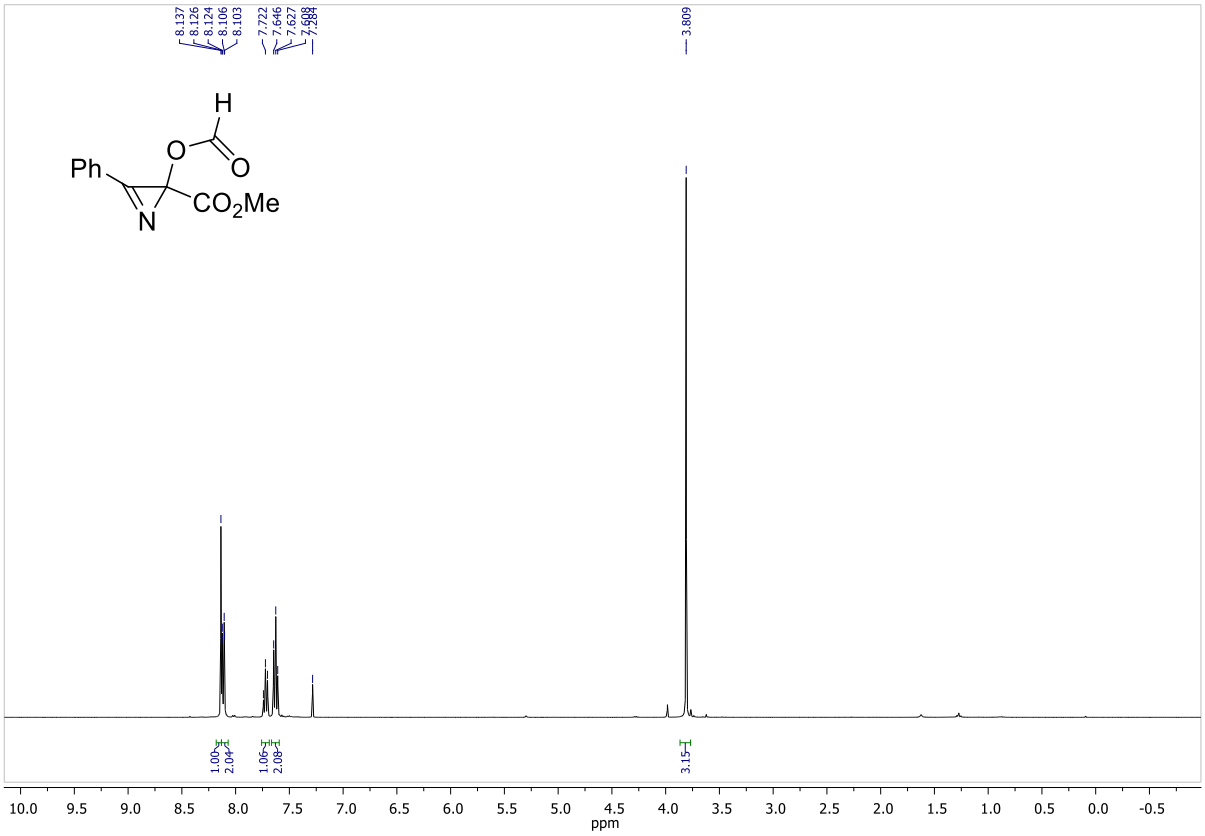


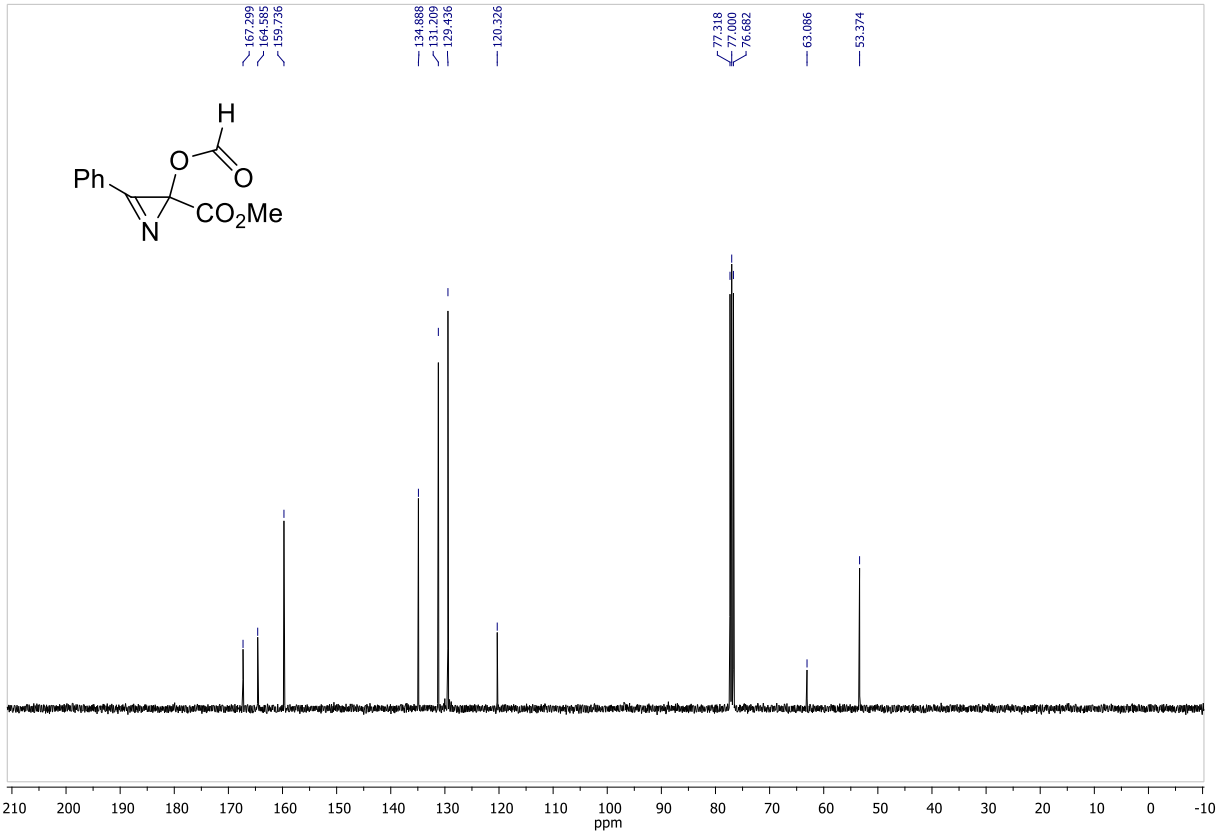
2-(Methoxycarbonyl)-3-phenyl-2*H*-azirin-2-yl isonicotinate (**2p**)



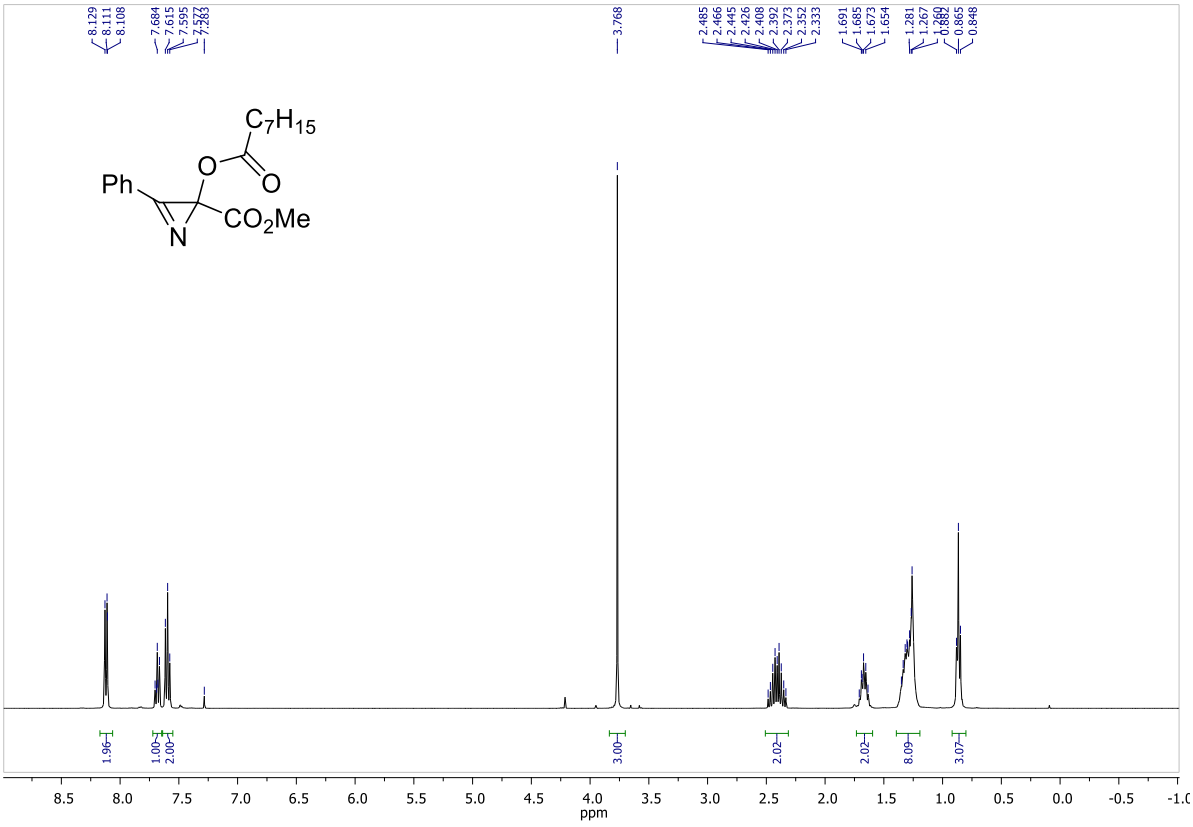


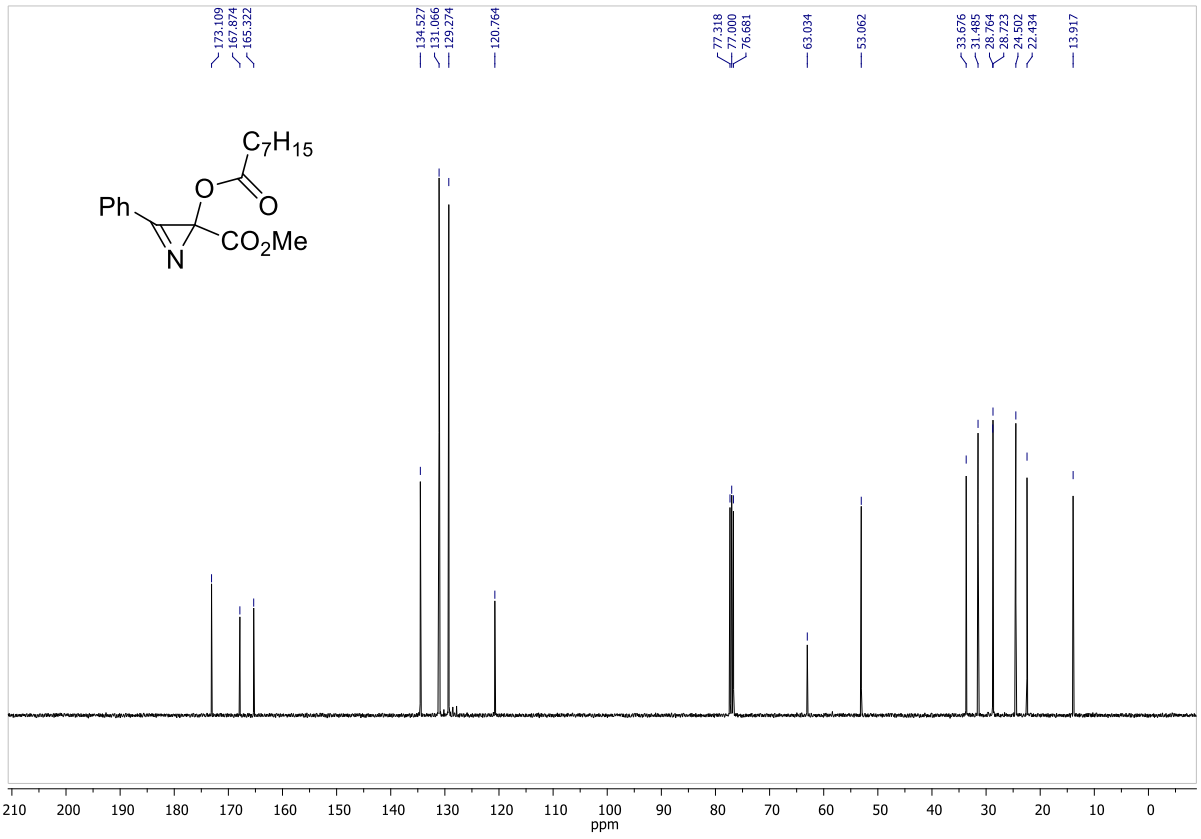
Methyl 2-(formyloxy)-3-phenyl-2*H*-azirine-2-carboxylate (**2q**)



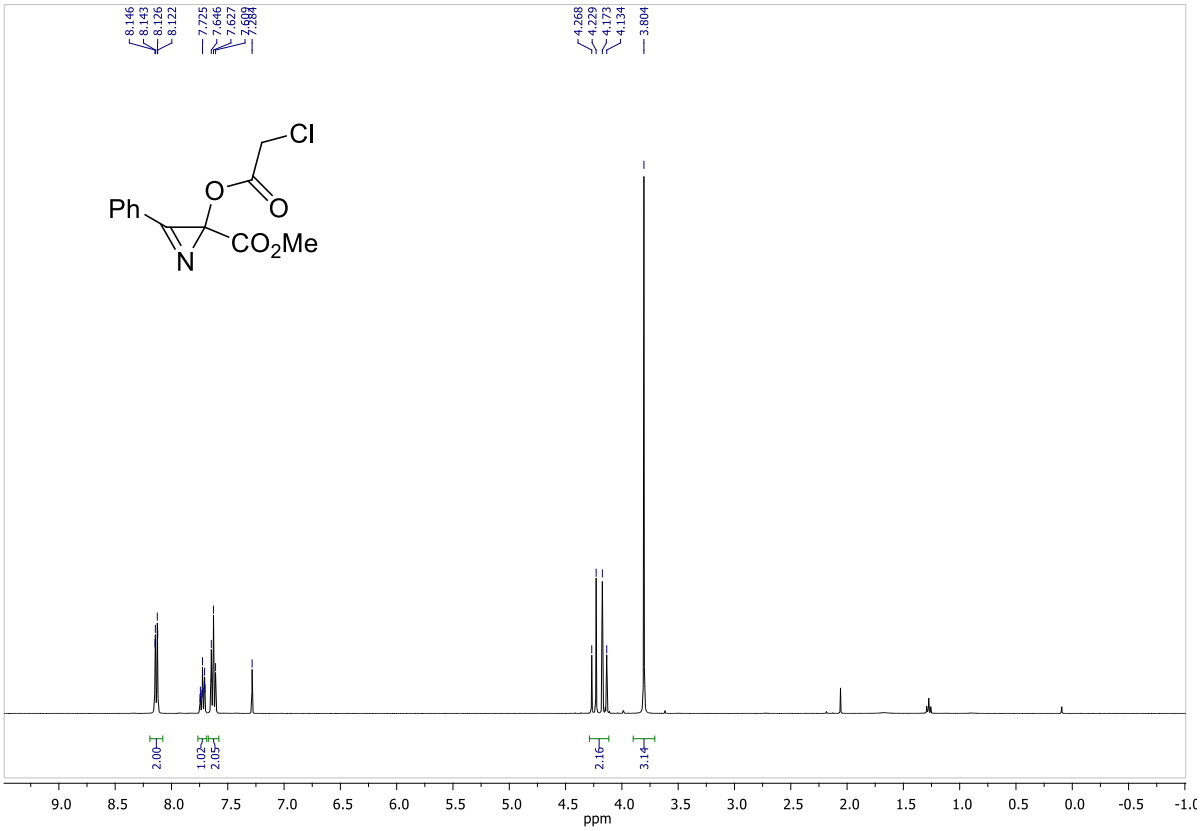


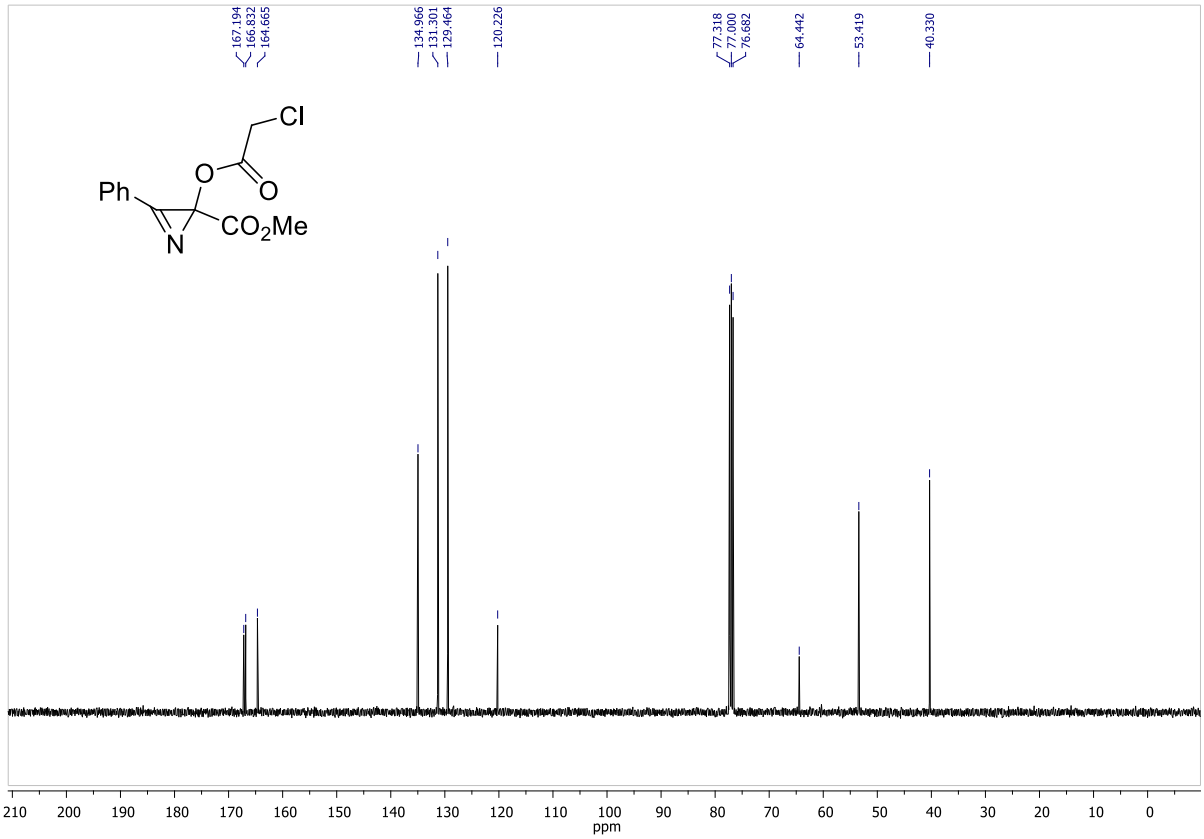
Methyl 2-(2-octanoyloxy)-3-phenyl-2*H*-azirine-2-carboxylate (**2r**)



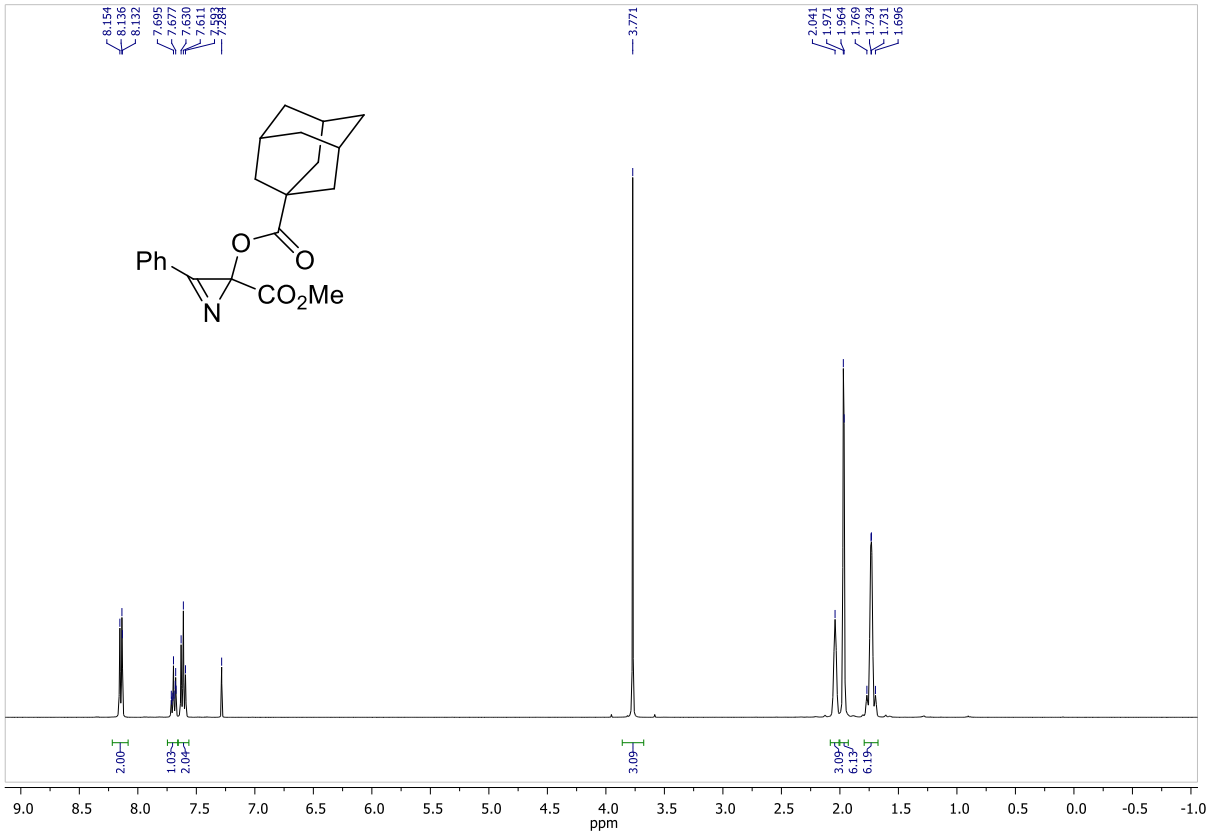


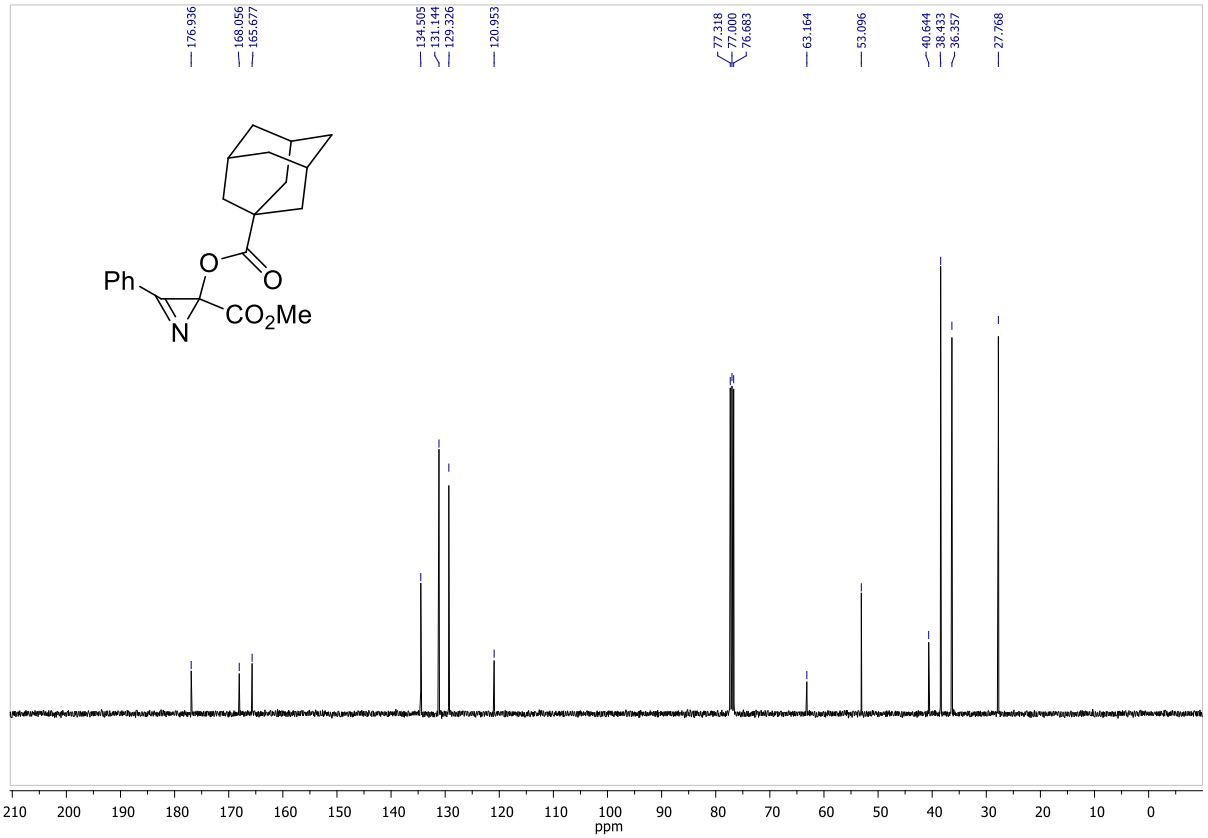
Methyl 2-(2-chloroacetoxy)-3-phenyl-2*H*-azirine-2-carboxylate (**2s**)



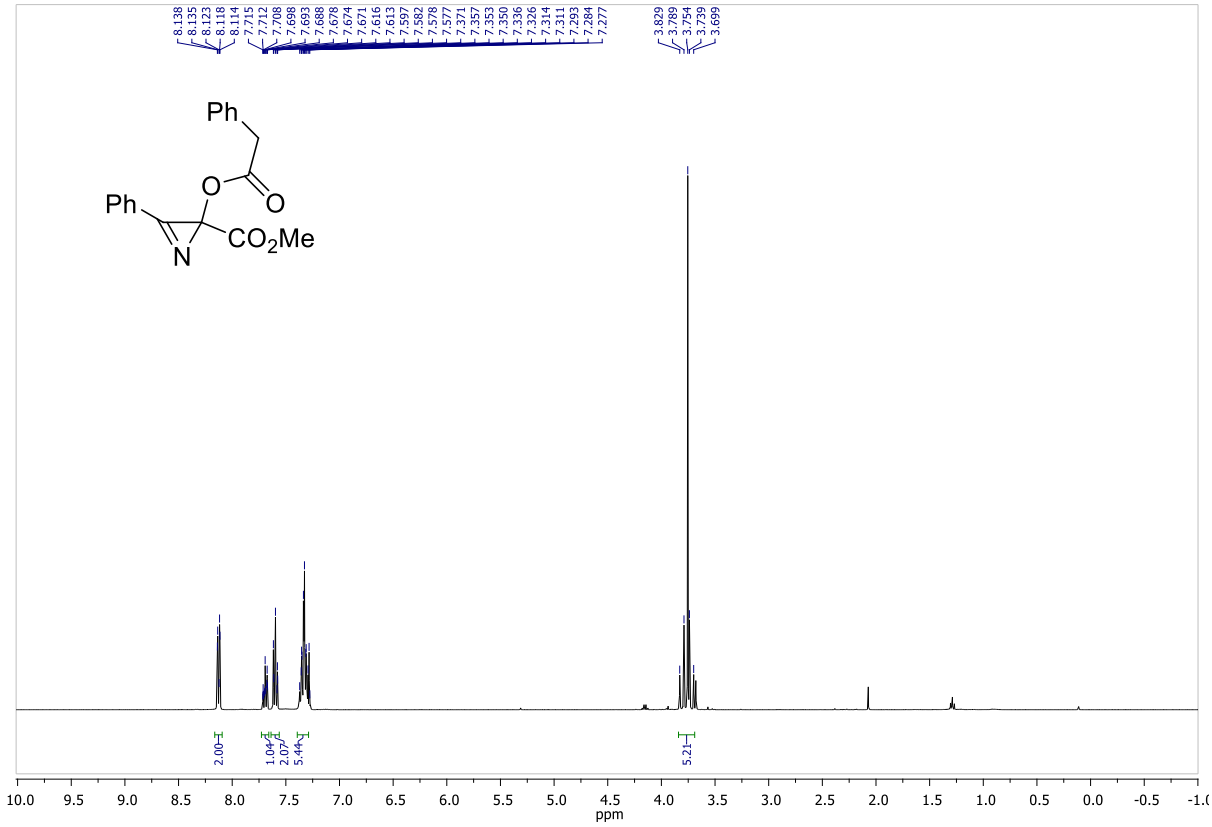


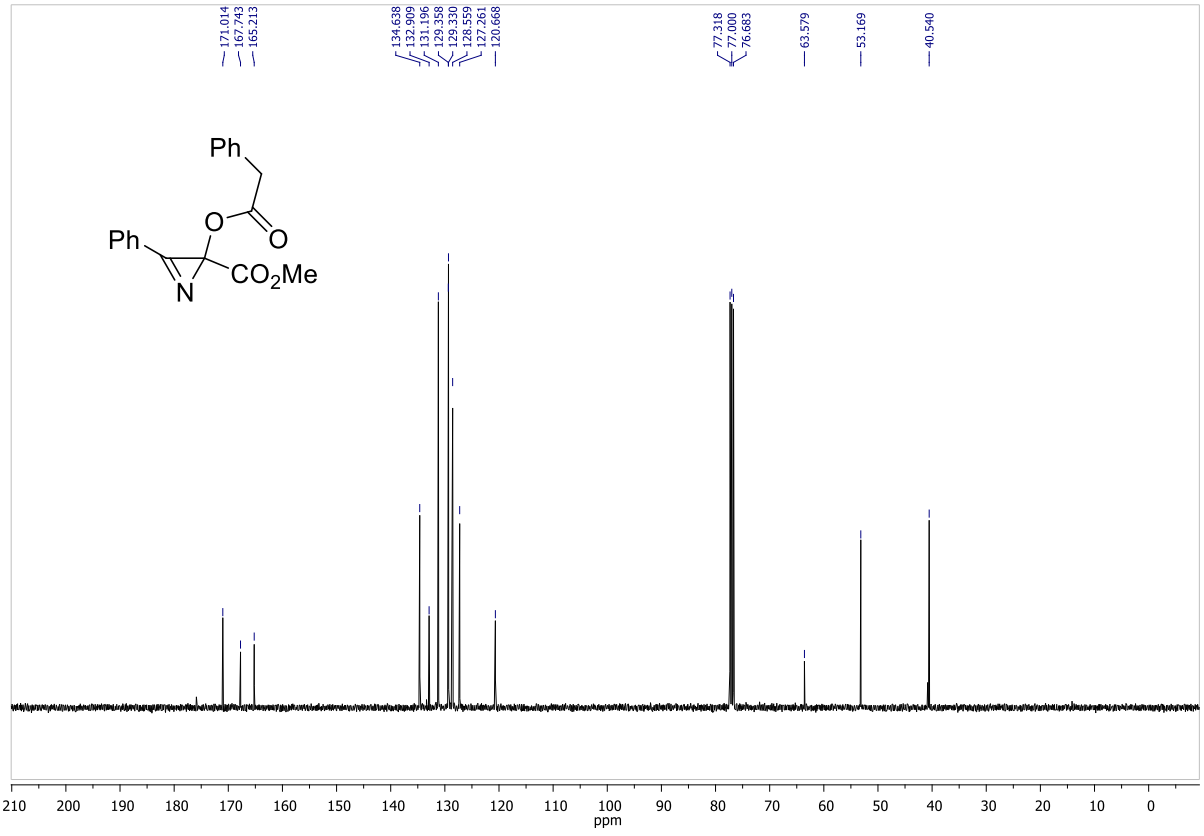
Methyl 2-(adamantan-1-carbonyloxy)-3-phenyl-2*H*-azirine-2-carboxylate (**2t**)



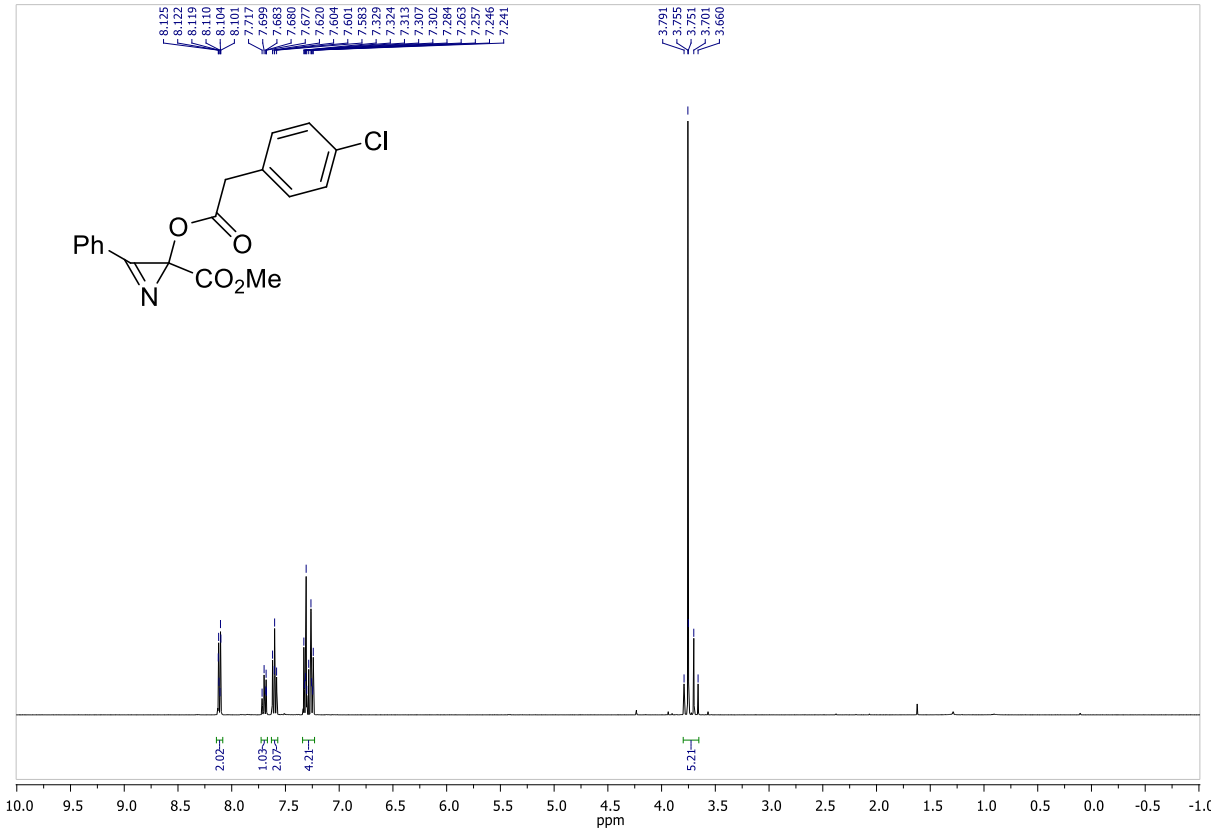


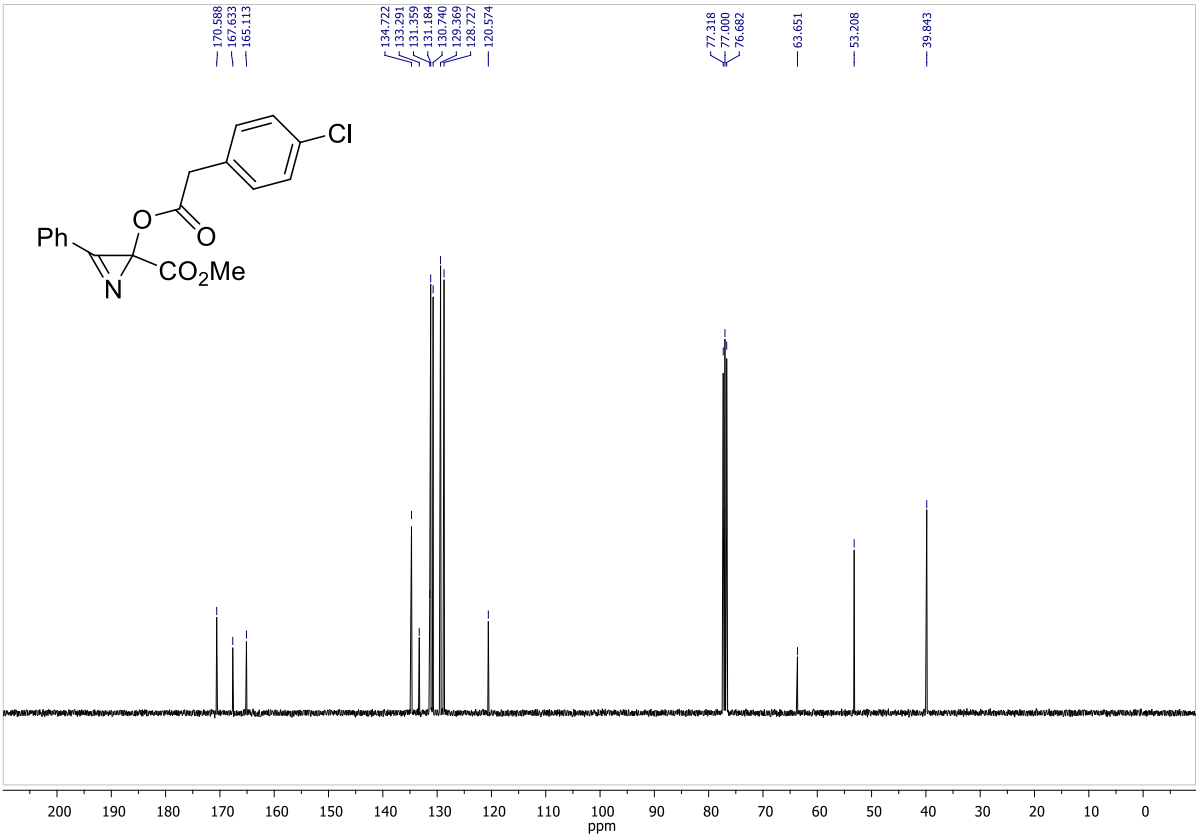
Methyl 3-phenyl-2-(2-phenylacetoxy)-2*H*-azirine-2-carboxylate (**2u**)



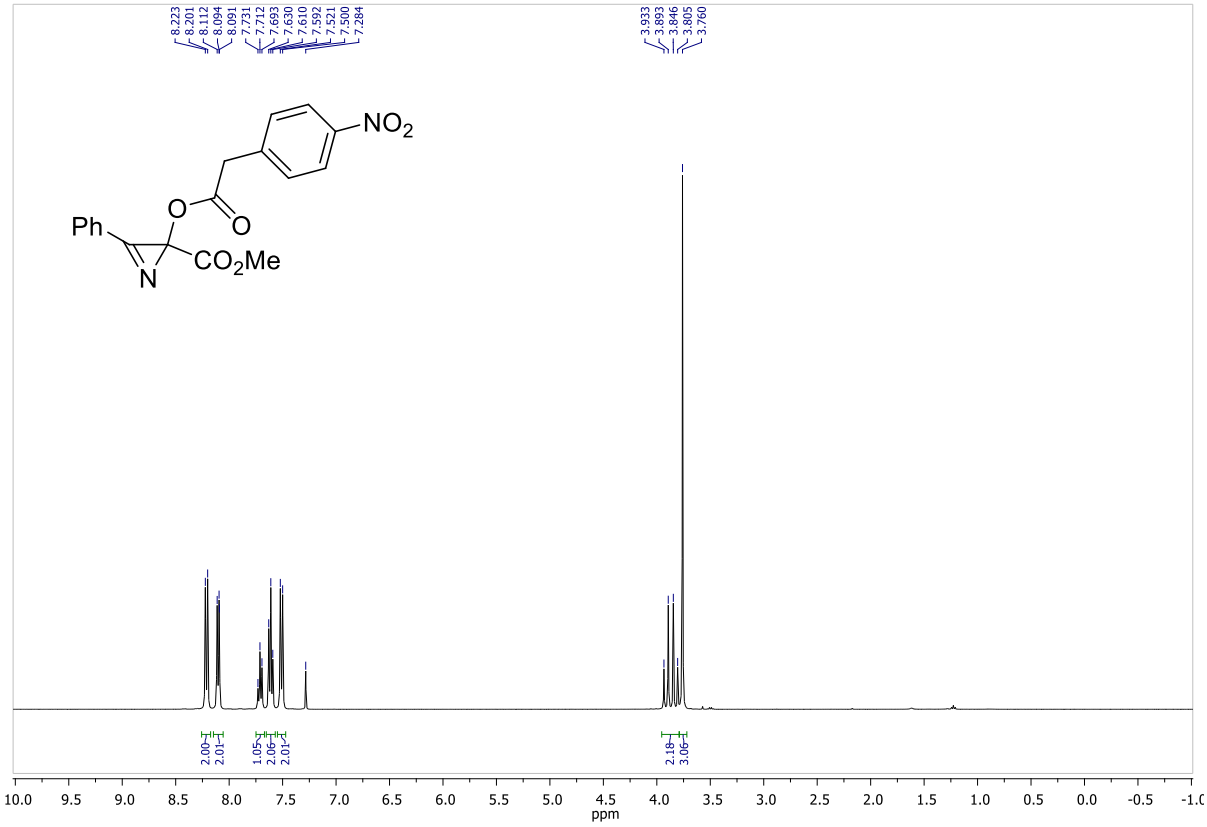


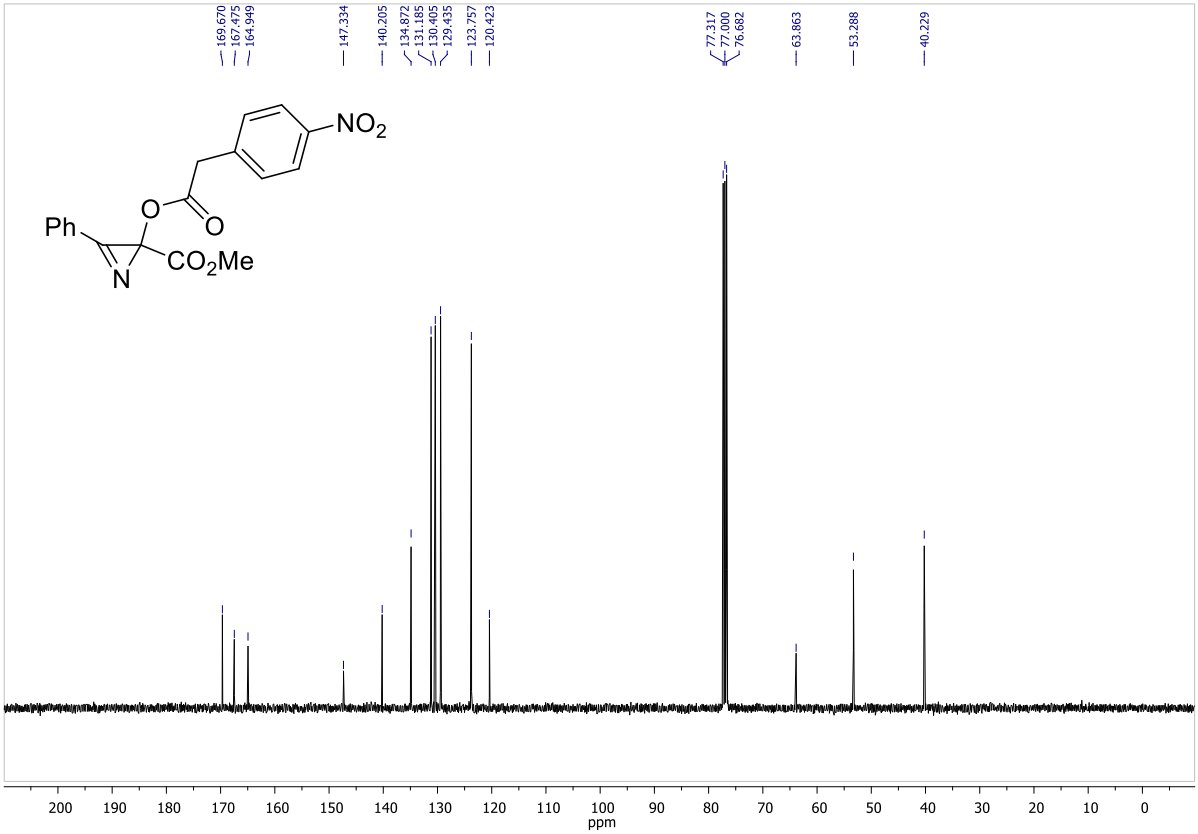
Methyl 2-(2-(4-chlorophenyl)acetoxy)-3-phenyl-2*H*-azirine-2-carboxylate (**2v**)



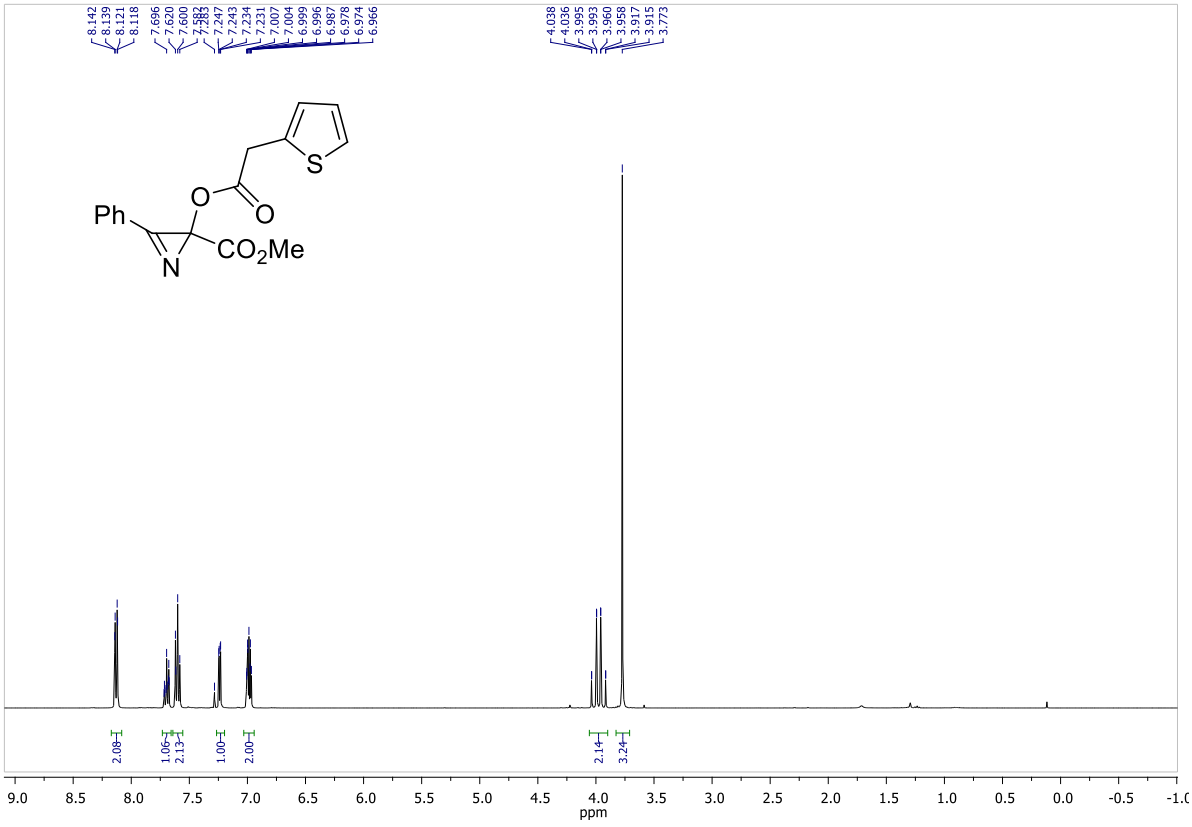


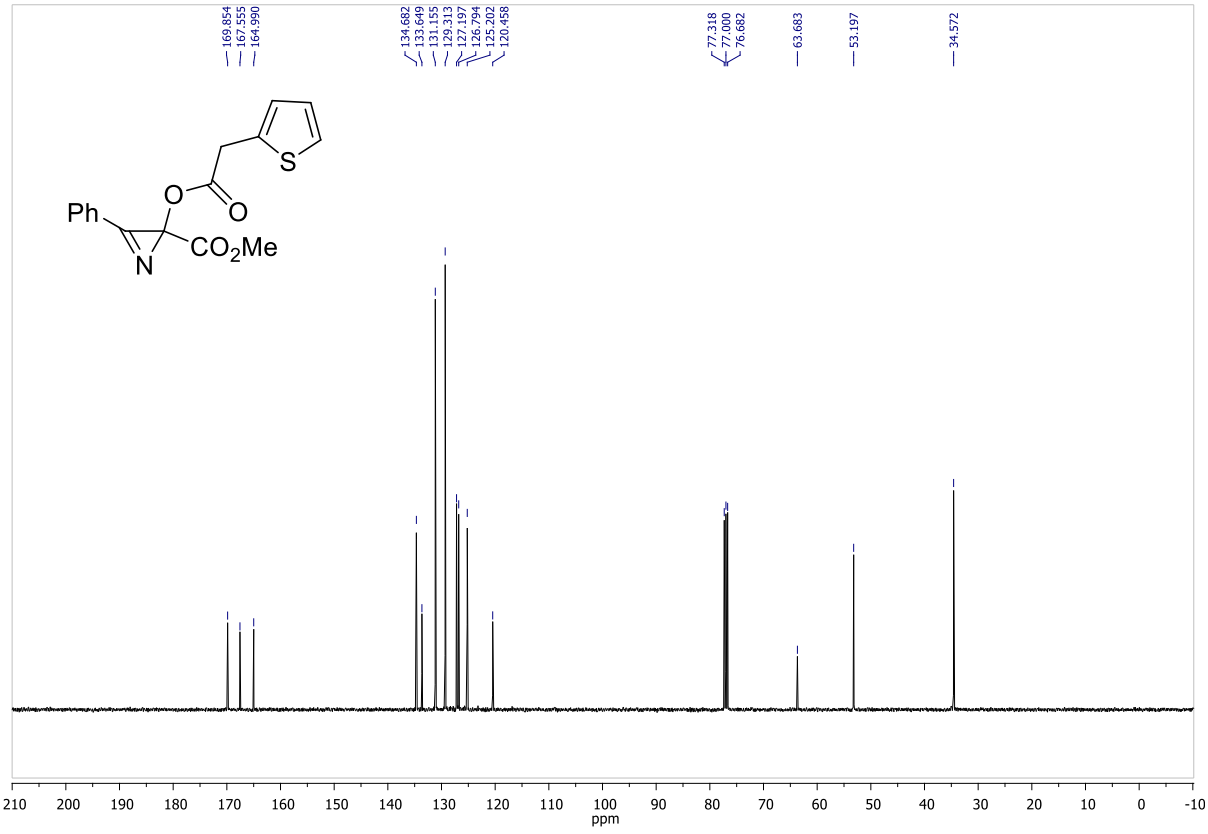
Methyl 2-[2-(4-nitrophenyl)acetoxy]-3-phenyl-2*H*-azirine-2-carboxylate (**2w**)



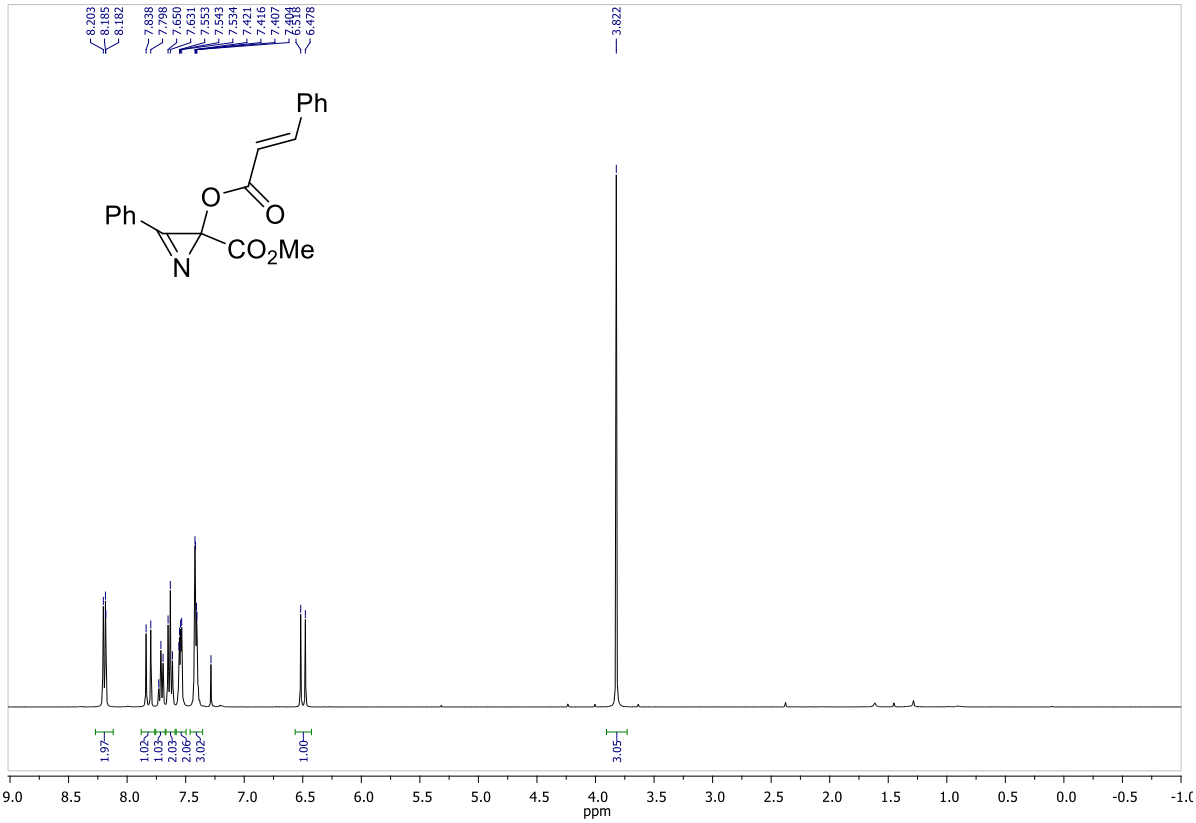


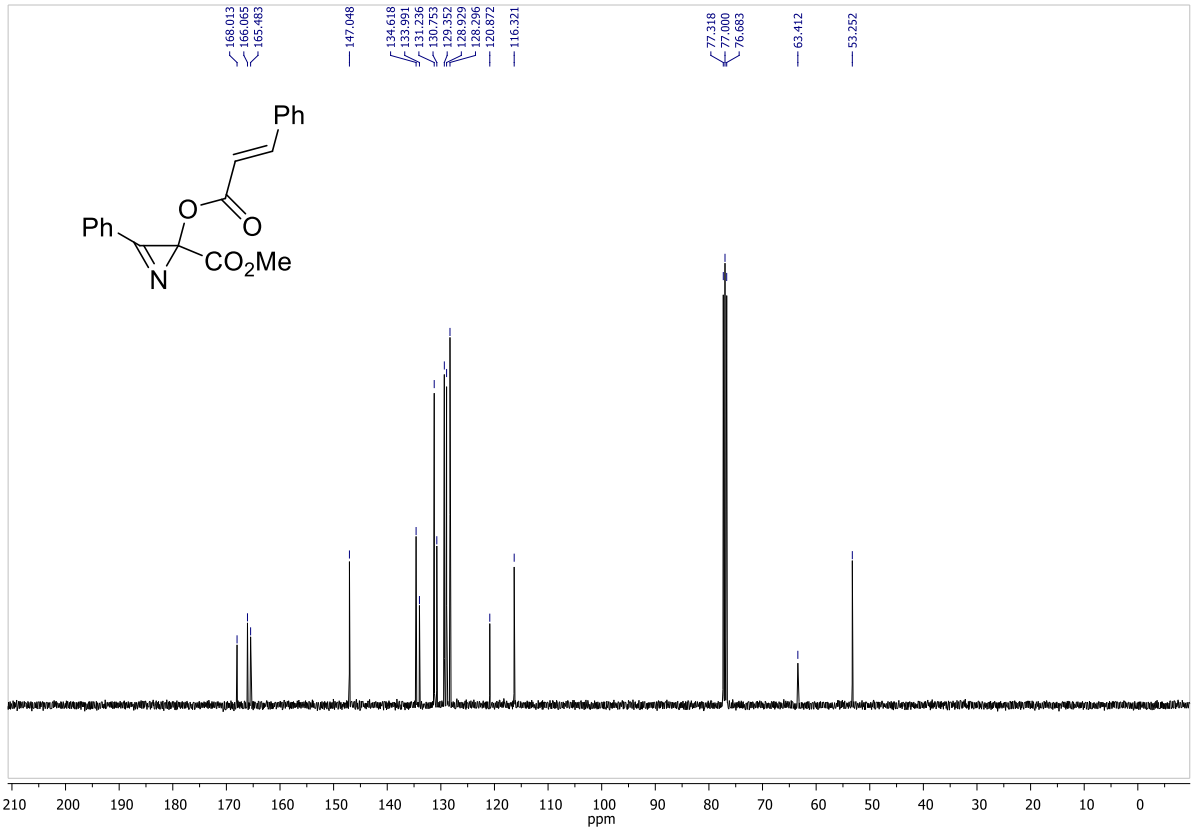
Methyl 3-phenyl-2-(2-(thiophen-2-yl)acetoxy)-2*H*-azirine-2-carboxylate (**2x**)



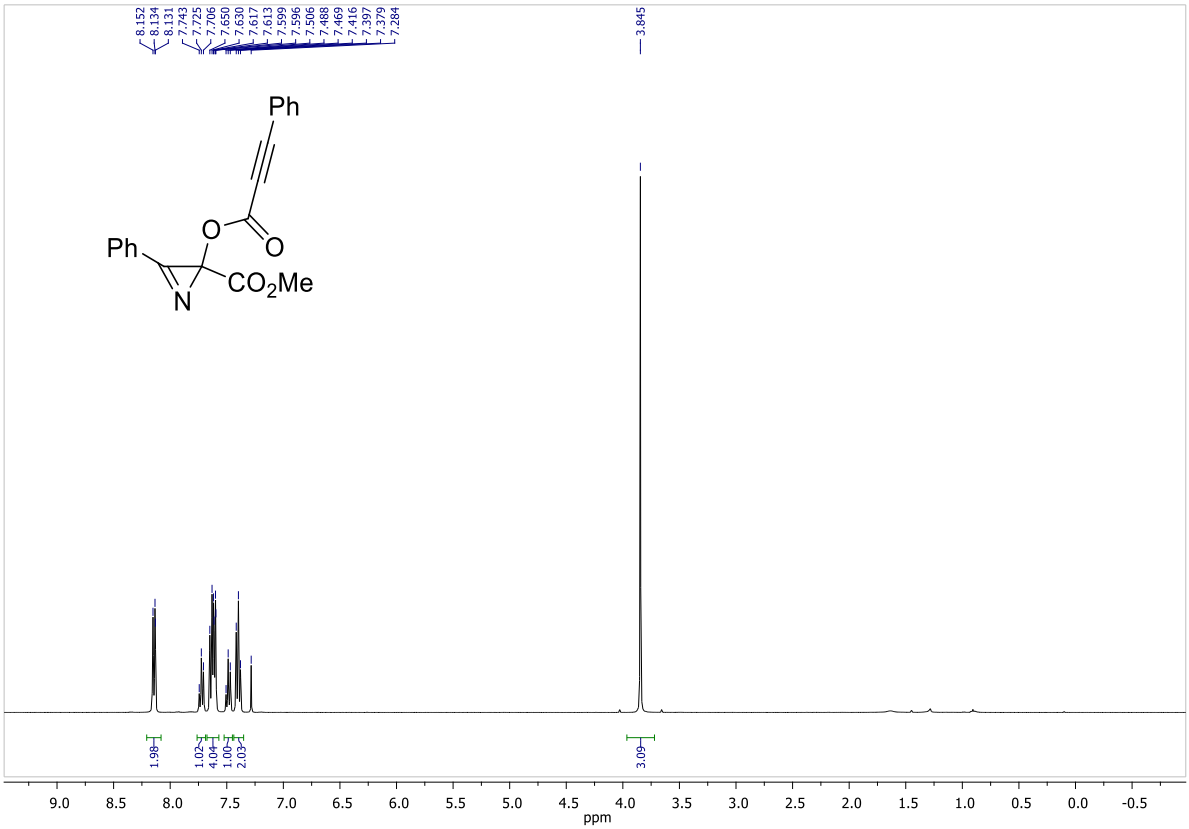


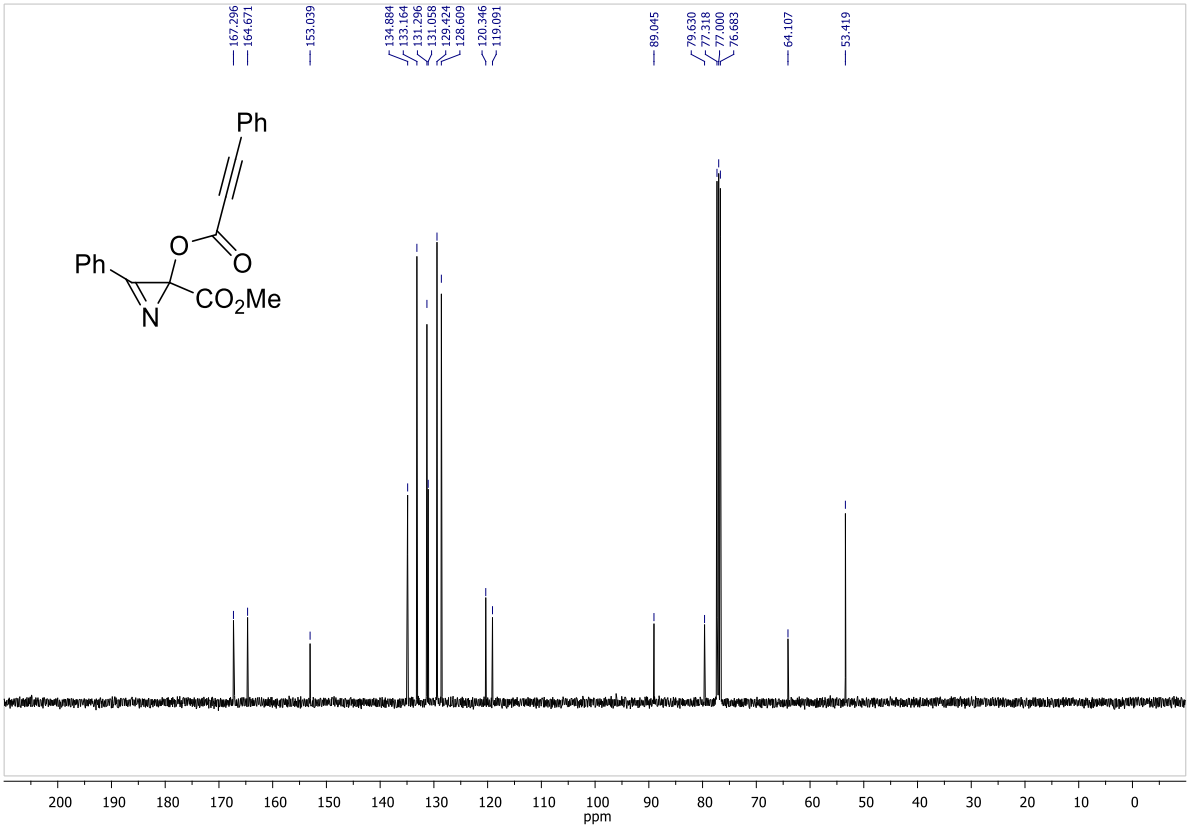
Methyl 2-(cinnamoyloxy)-3-phenyl-2*H*-azirine-2-carboxylate (**2y**)



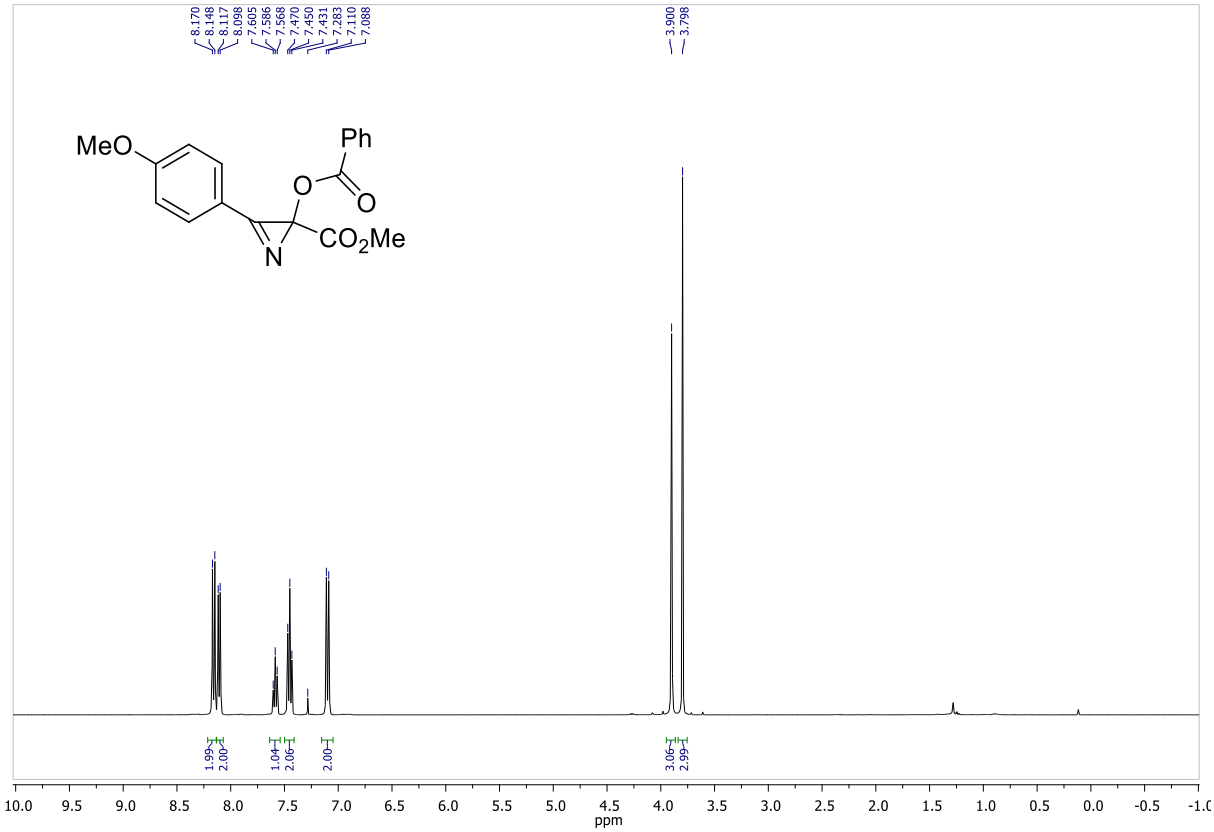


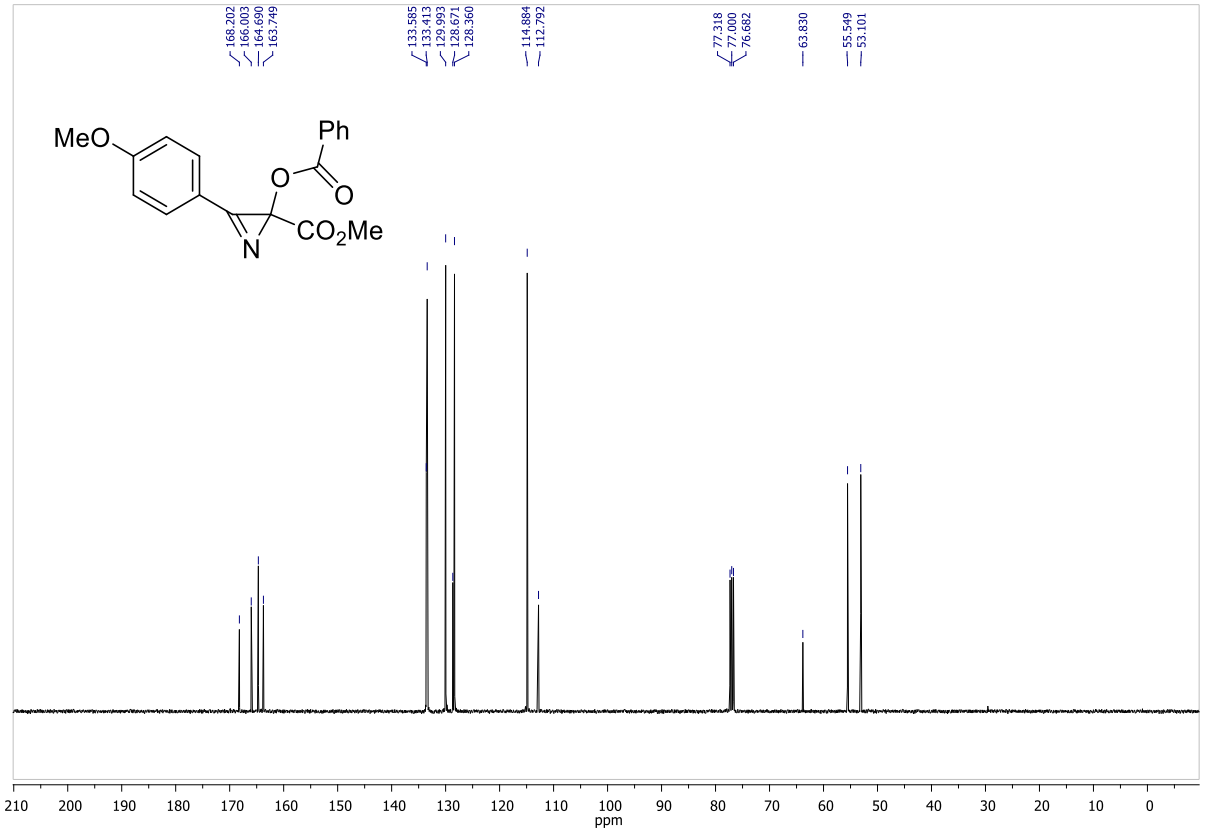
Methyl 3-phenyl-2-(3-phenylpropioloyloxy)-2*H*-azirine-2-carboxylate (**2z**)



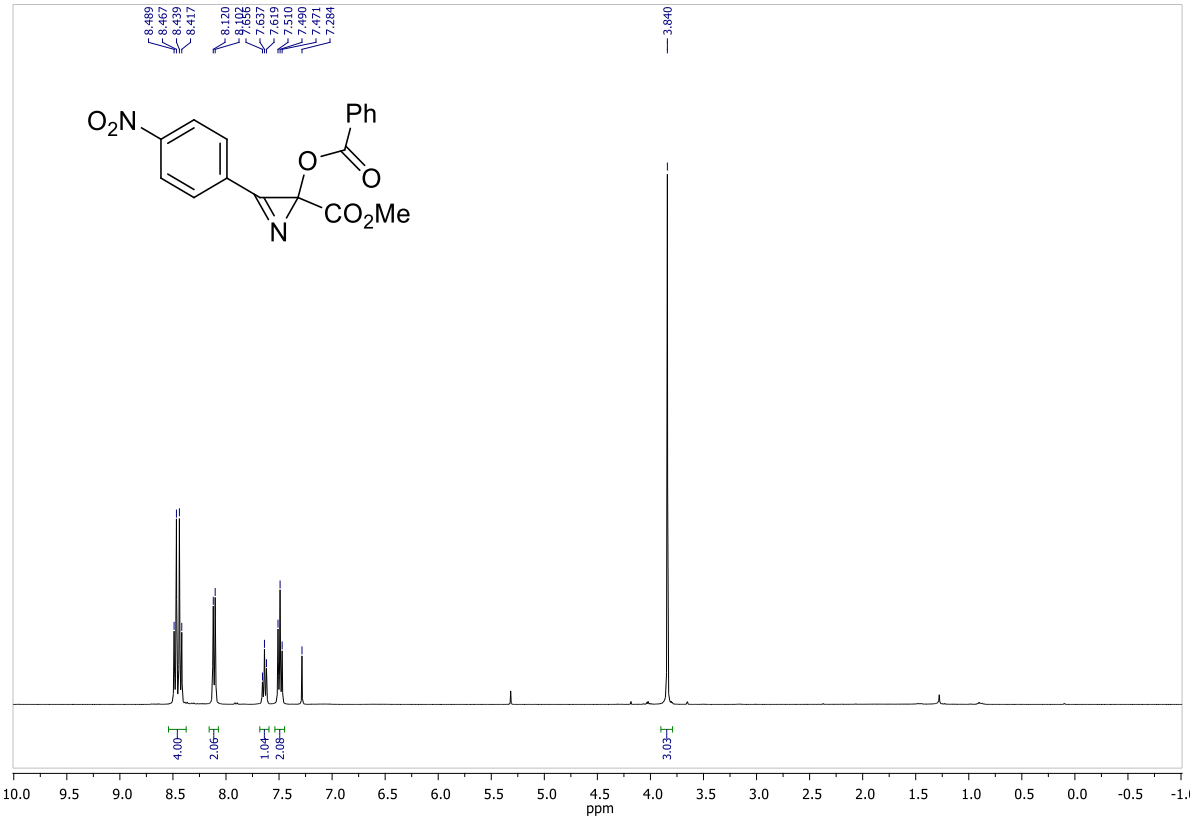


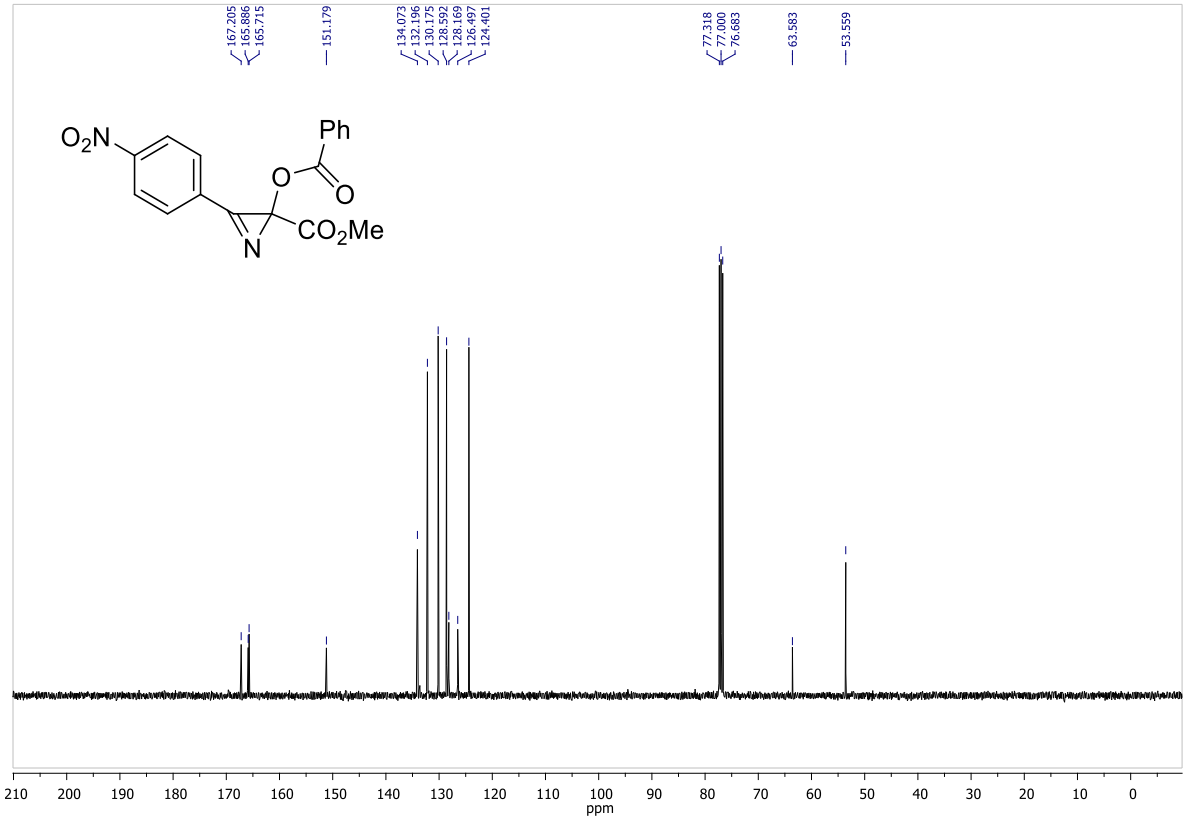
Methyl 2-(benzoyloxy)-3-(4-methoxyphenyl)-2*H*-azirine-2-carboxylate (**2za**)



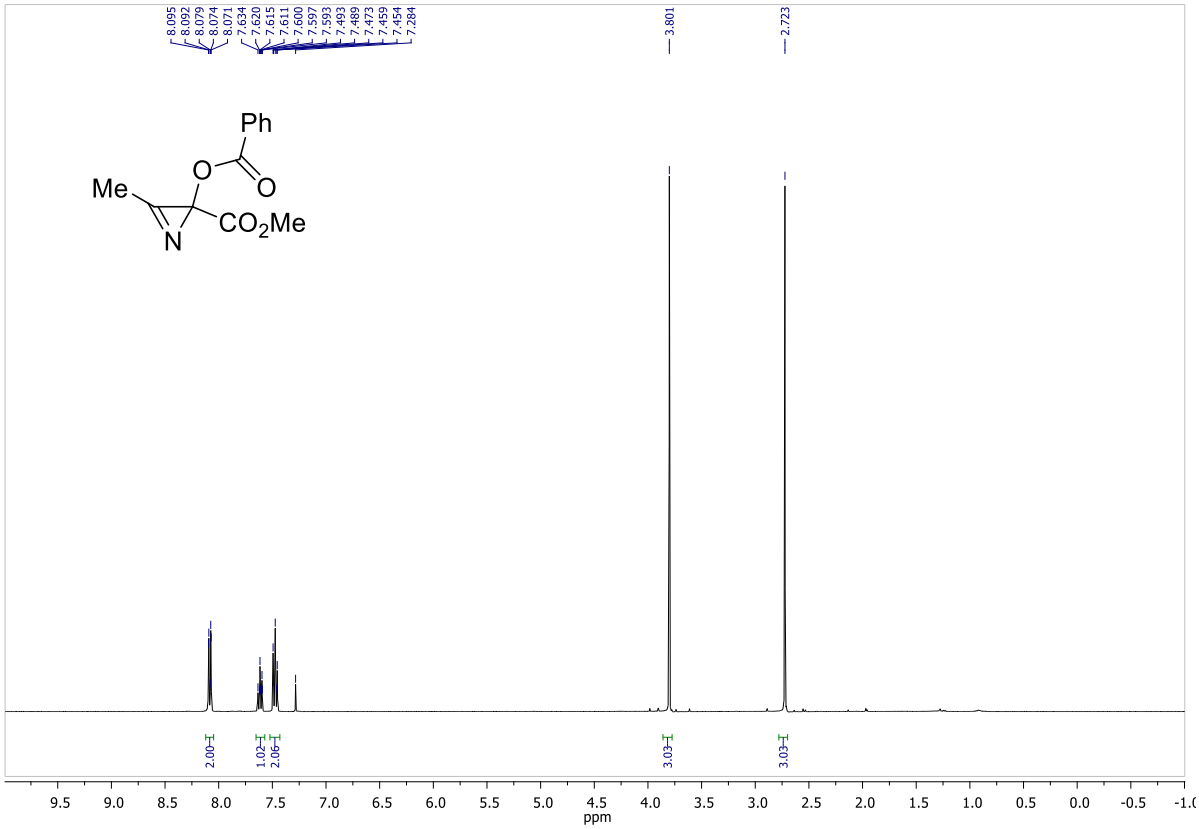


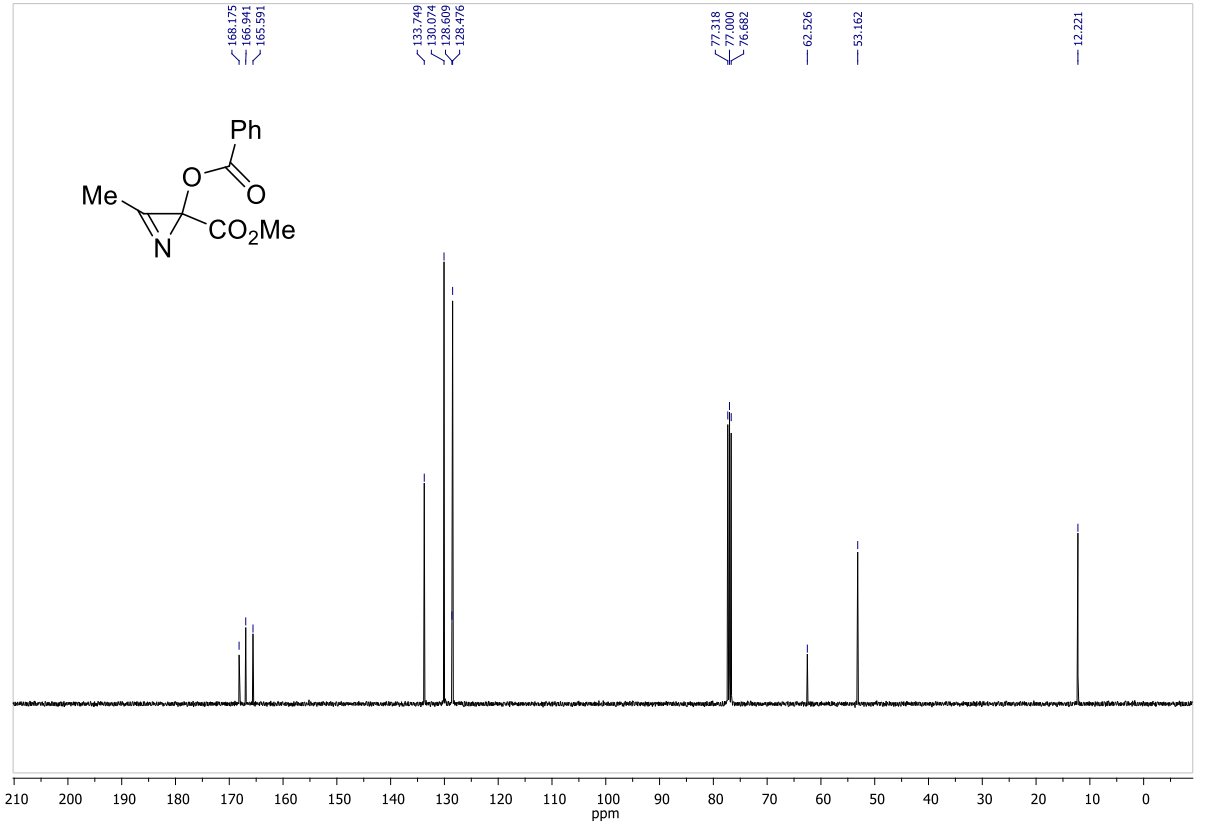
Methyl 2-(benzoyloxy)-3-(4-nitrophenyl)-2*H*-azirine-2-carboxylate (**2zb**)



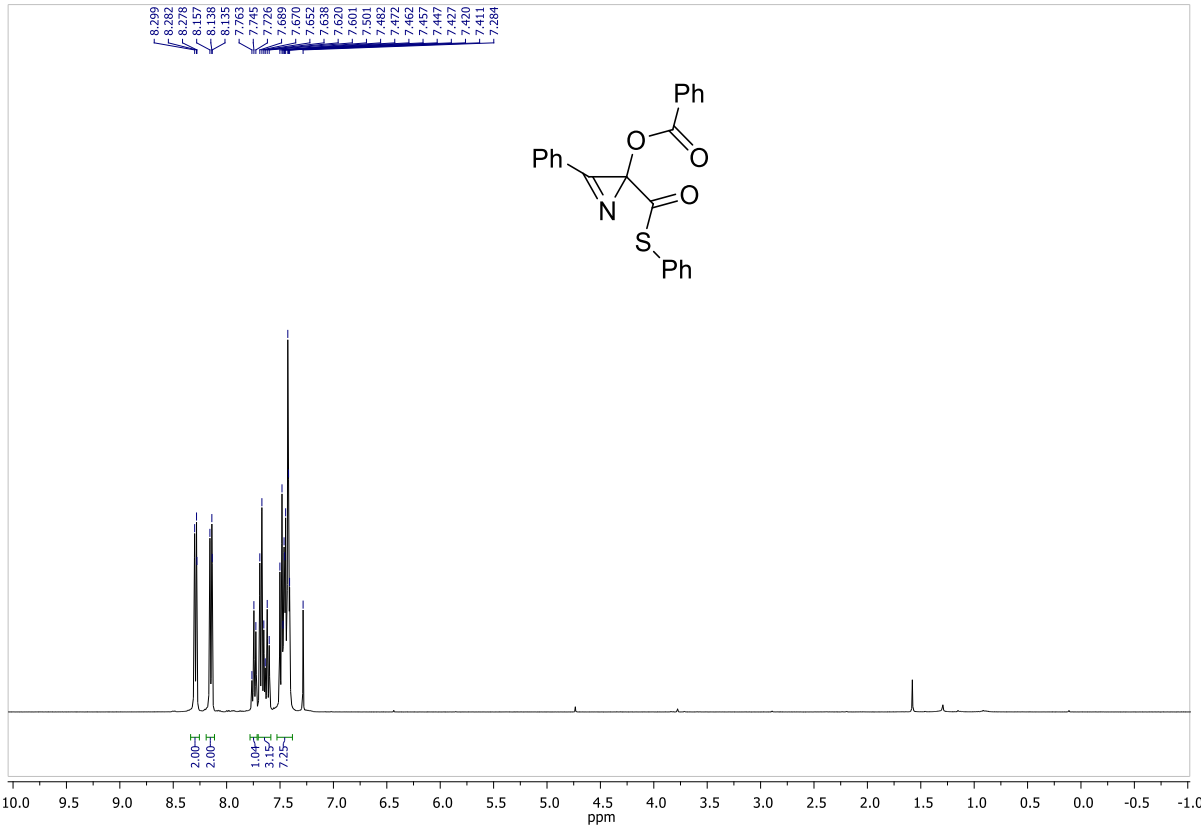


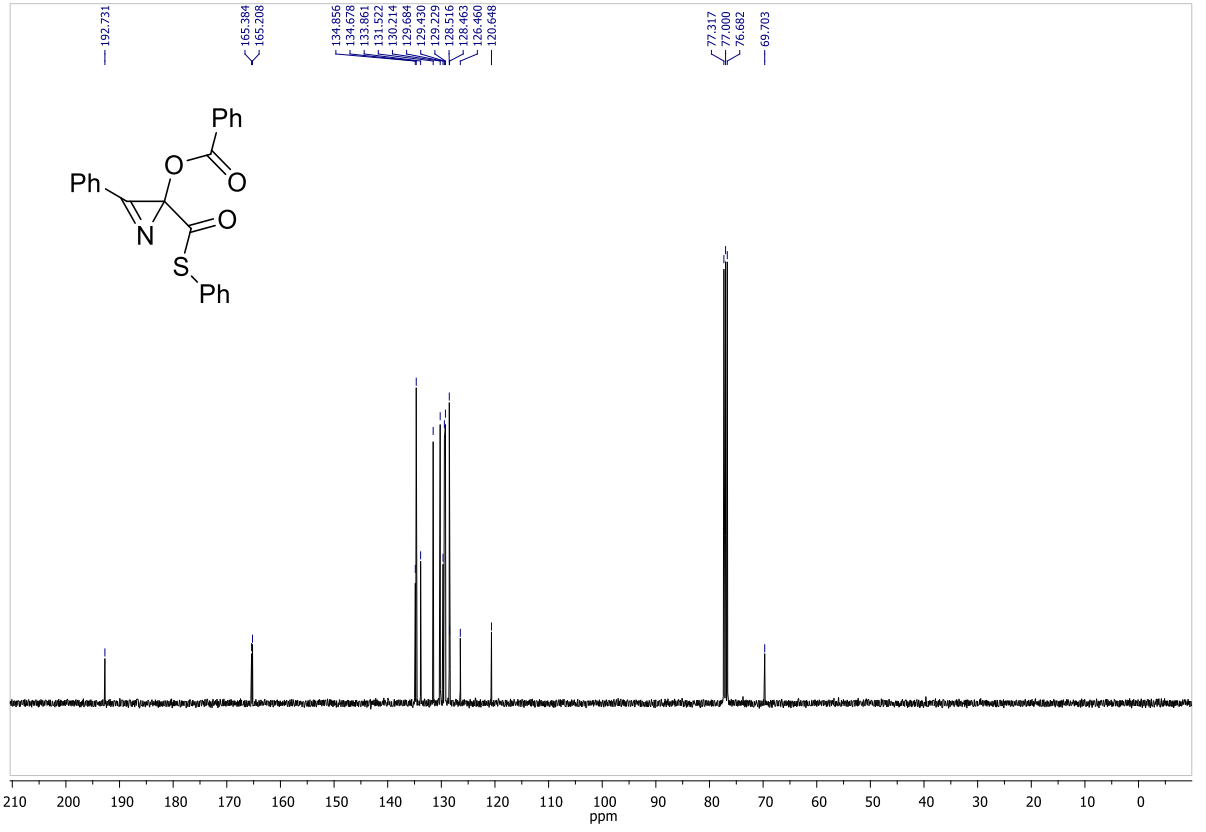
Methyl 2-(benzoyloxy)-3-methyl-2*H*-azirine-2-carboxylate (**2zc**)



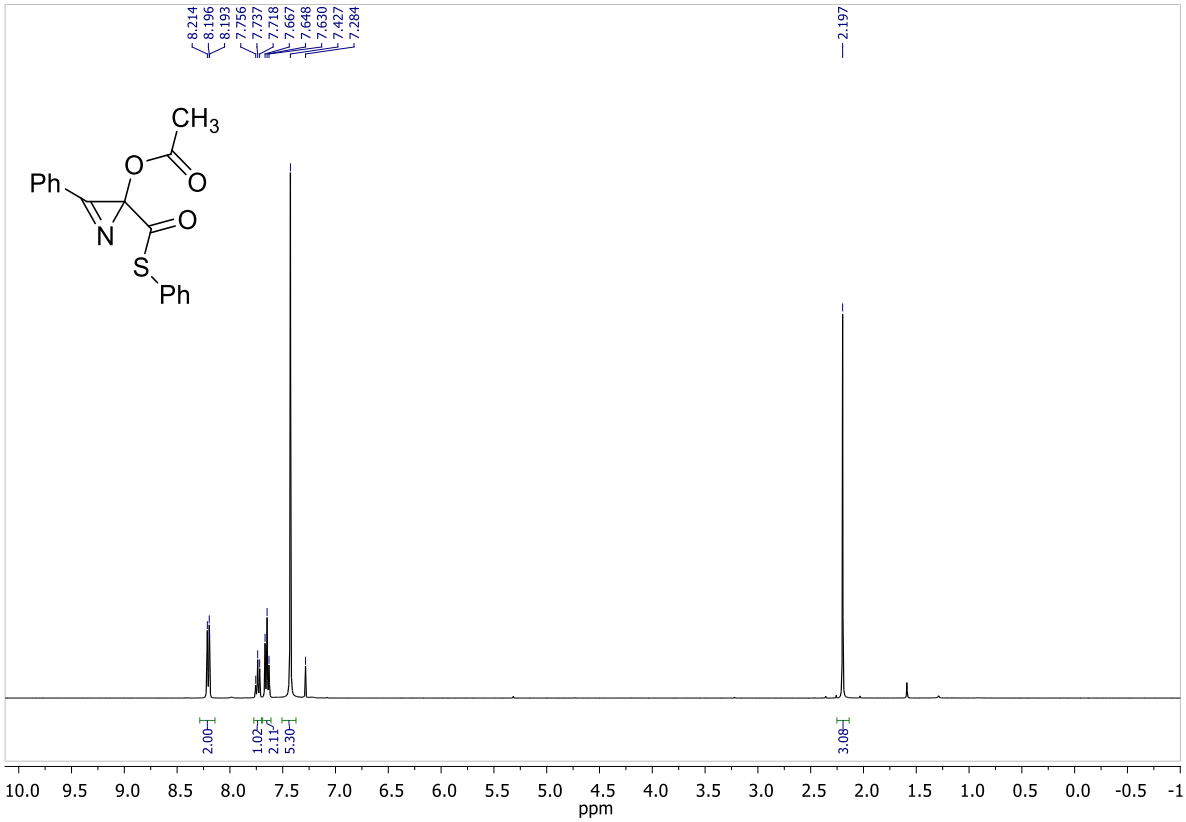


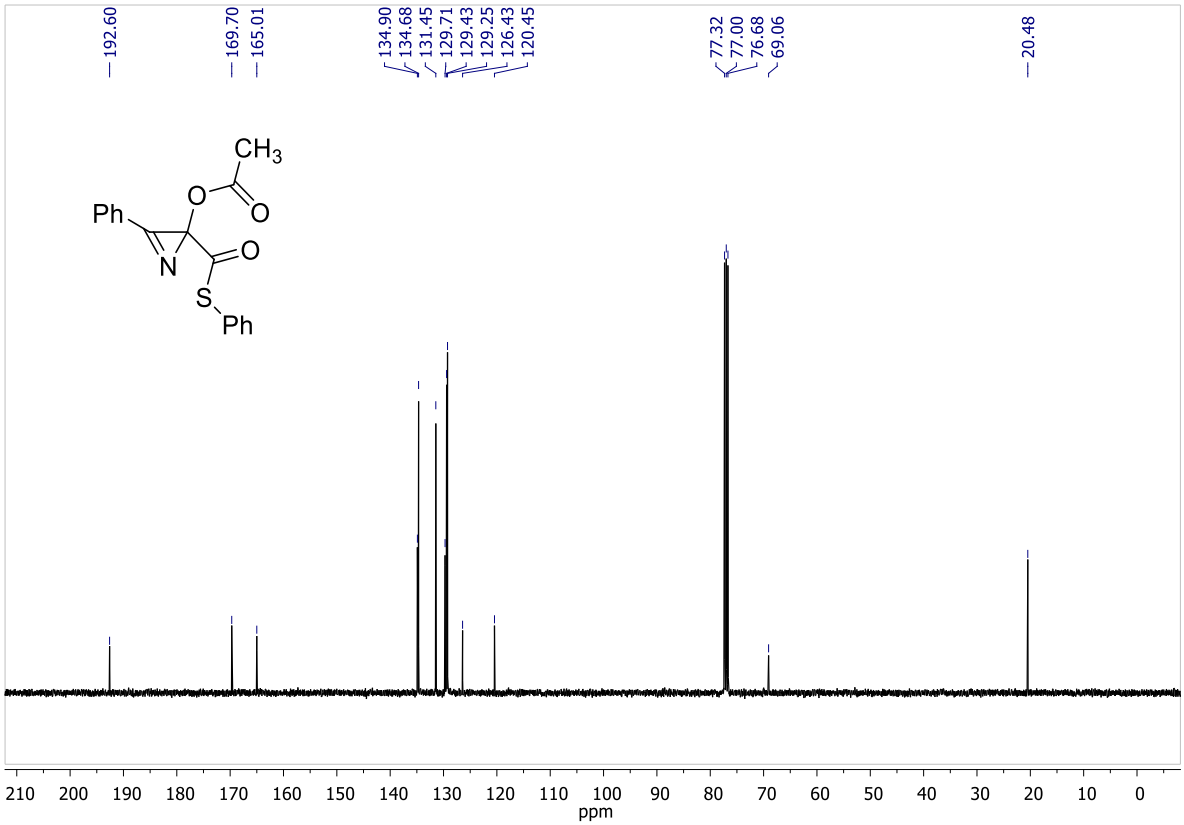
3-Phenyl-2-((phenylthio)carbonyl)-2*H*-azirin-2-yl benzoate (**2zd**)



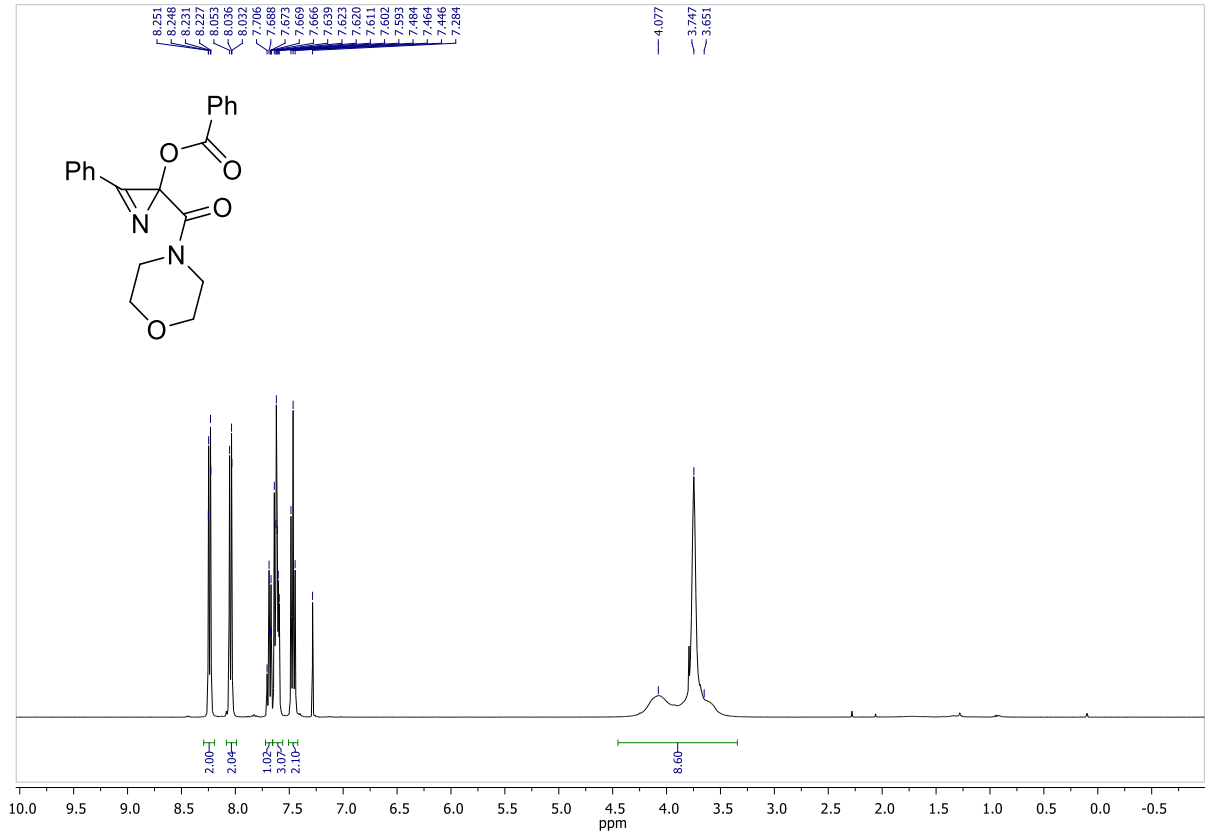


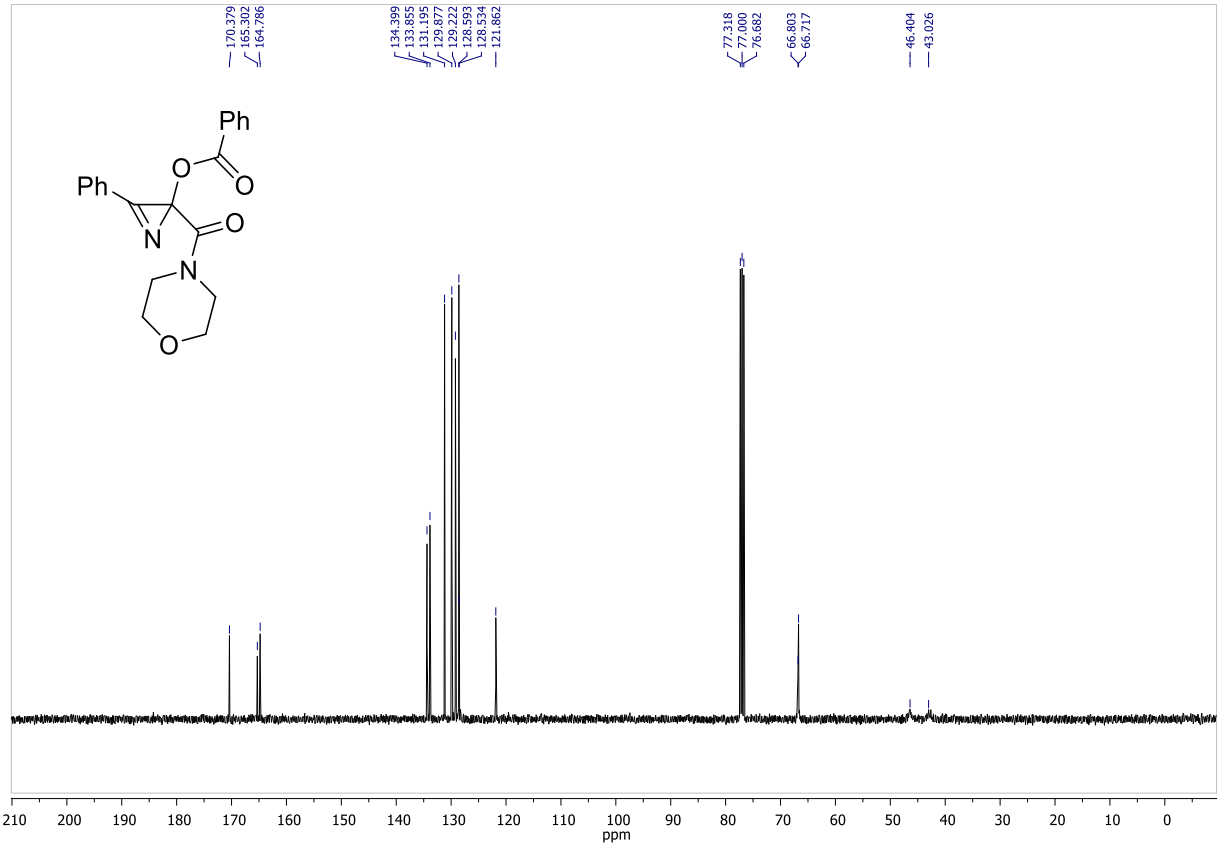
3-Phenyl-2-(phenylthiocarbonyl)-2*H*-azirin-2-yl acetate (**2ze**)



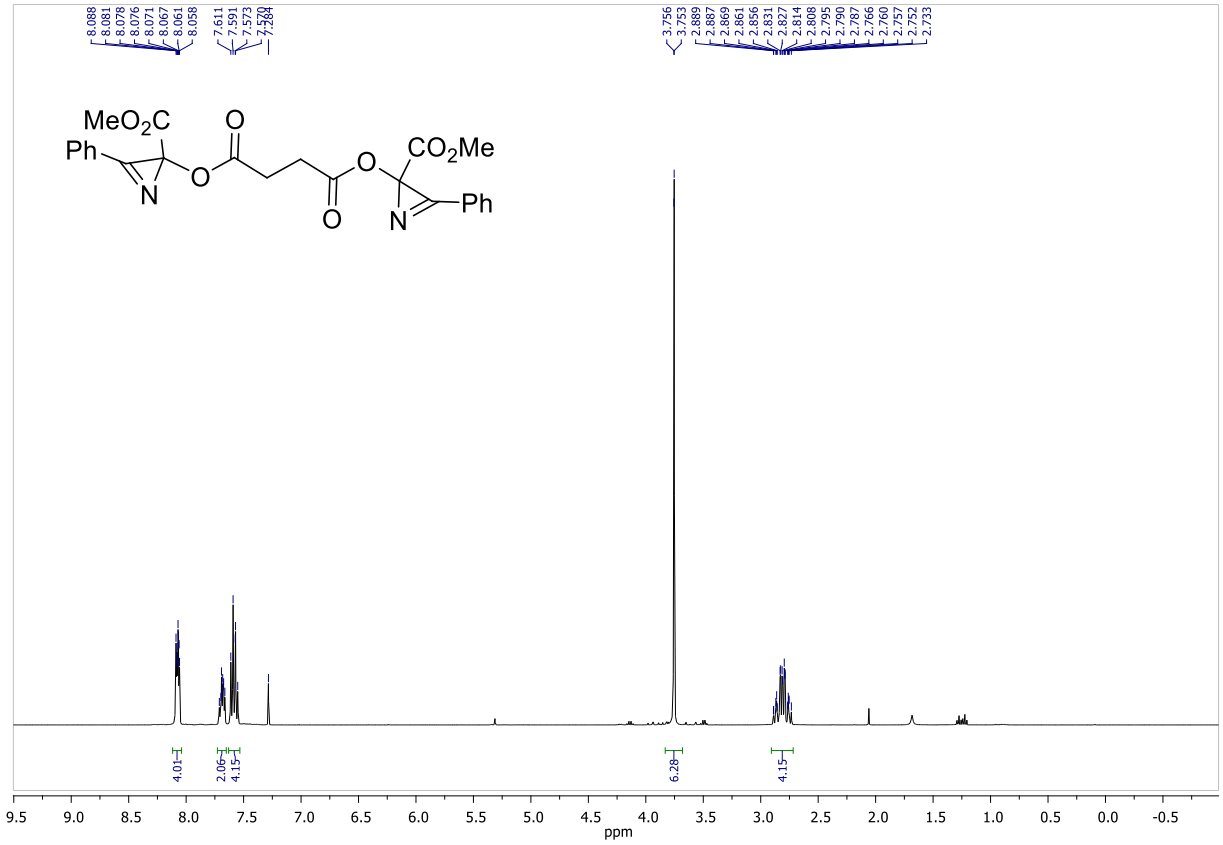


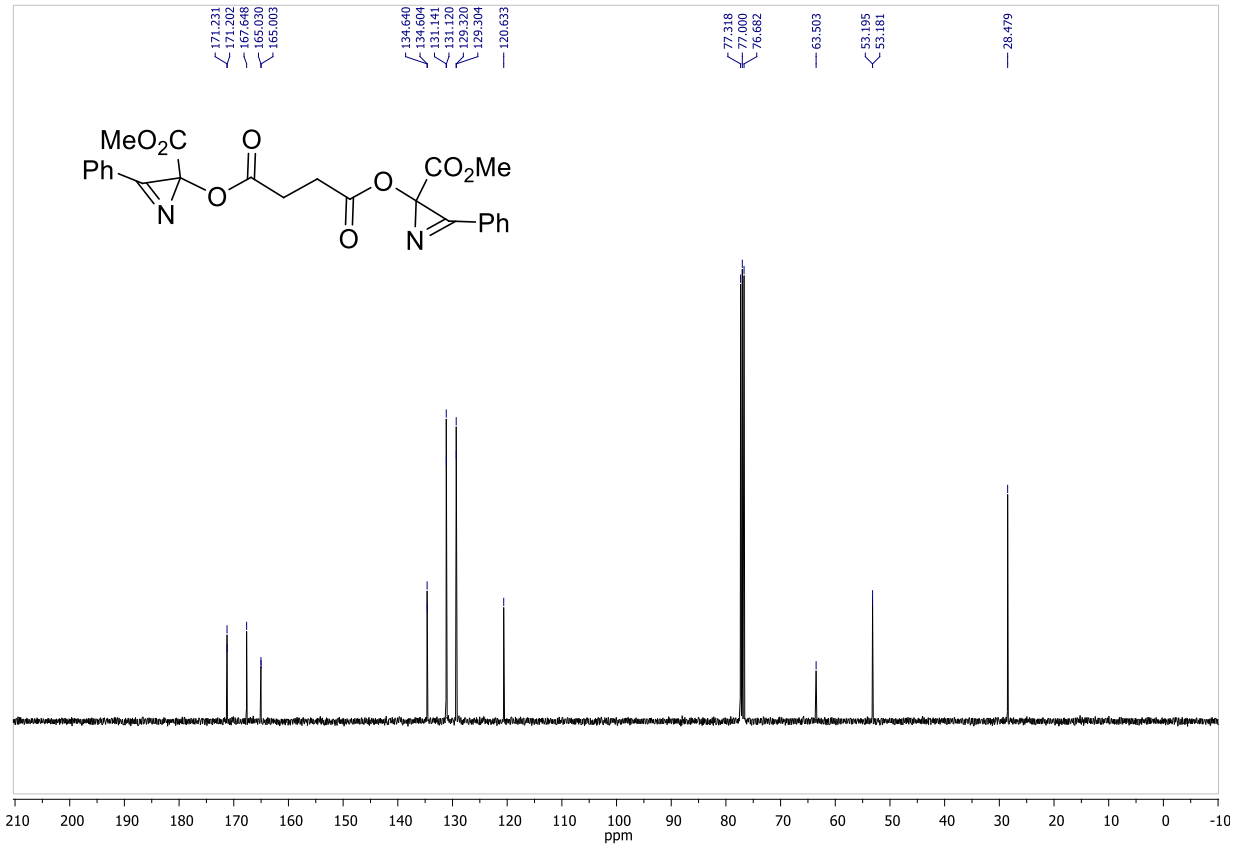
2-(Morpholine-4-carbonyl)-3-phenyl-2*H*-azirin-2-yl benzoate (**2zf)**



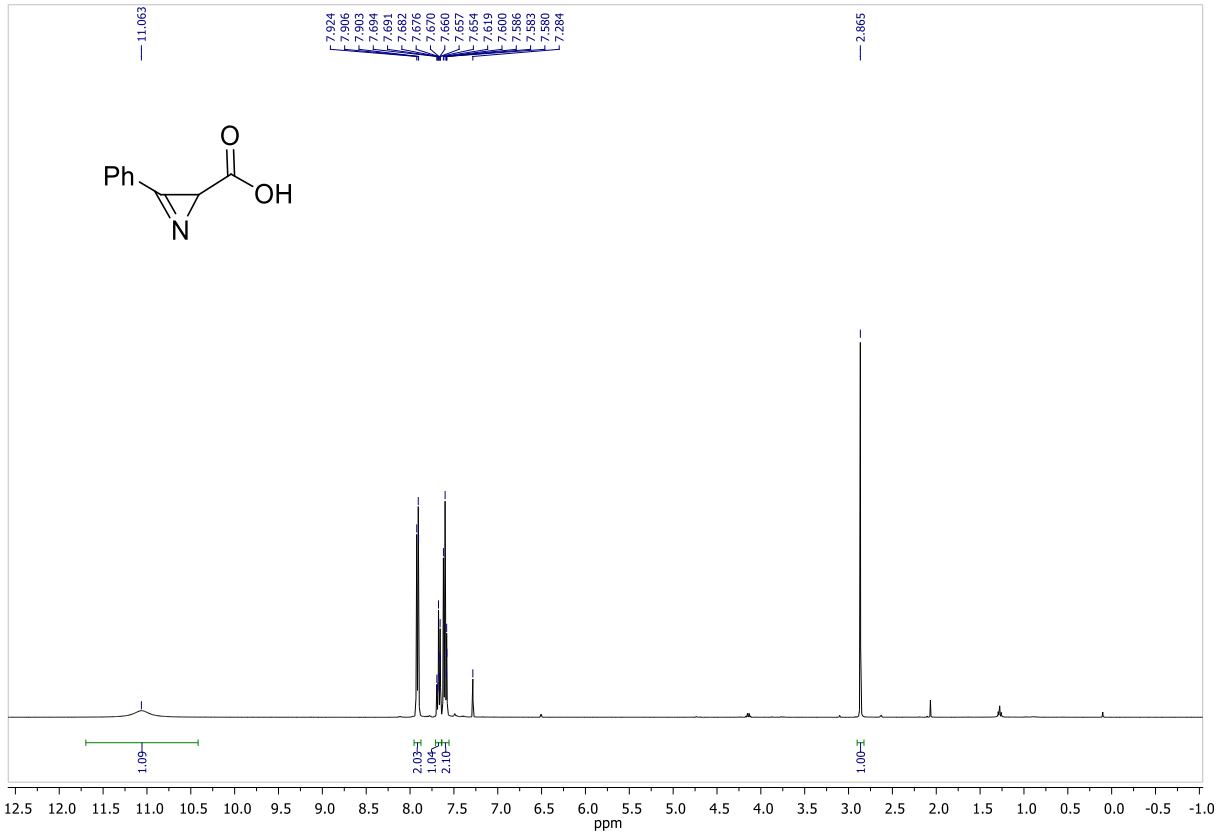


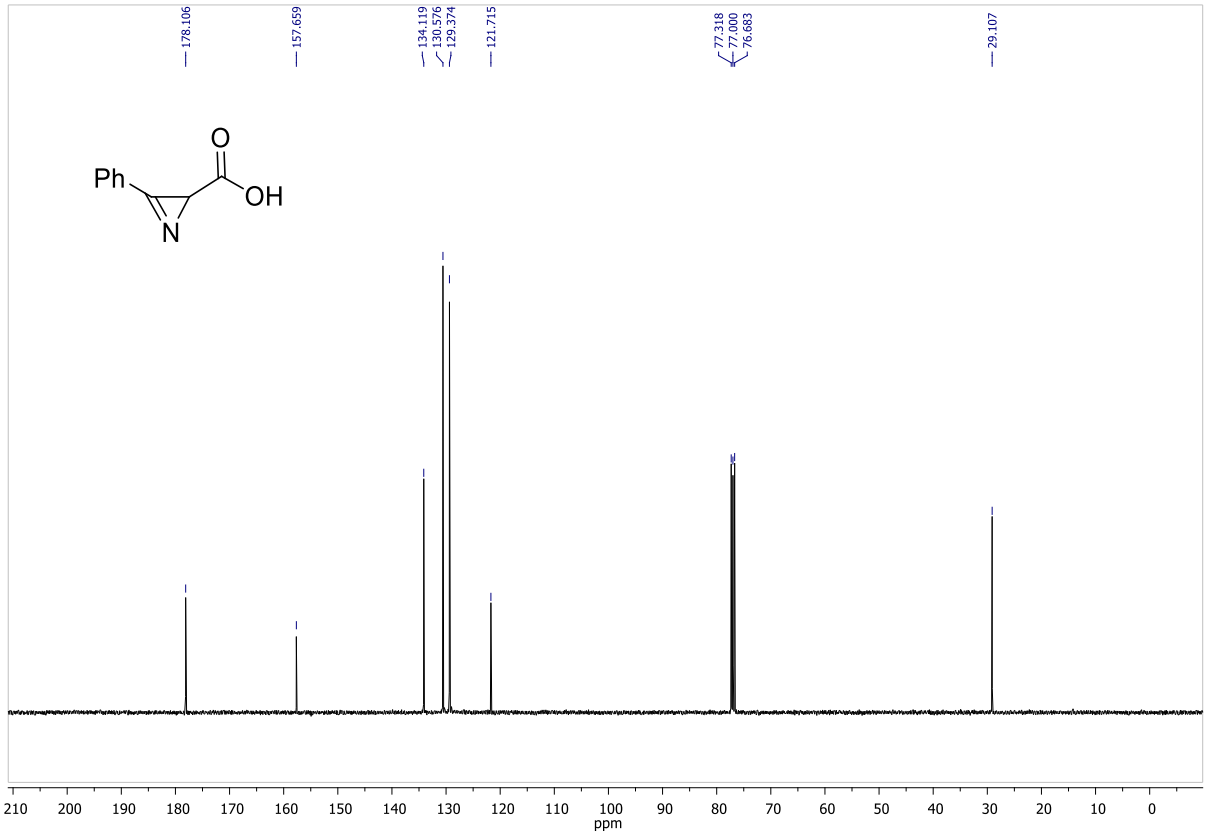
Bis[2-(methoxycarbonyl)-3-phenyl-2*H*-azirin-2-yl] succinate (**3**)



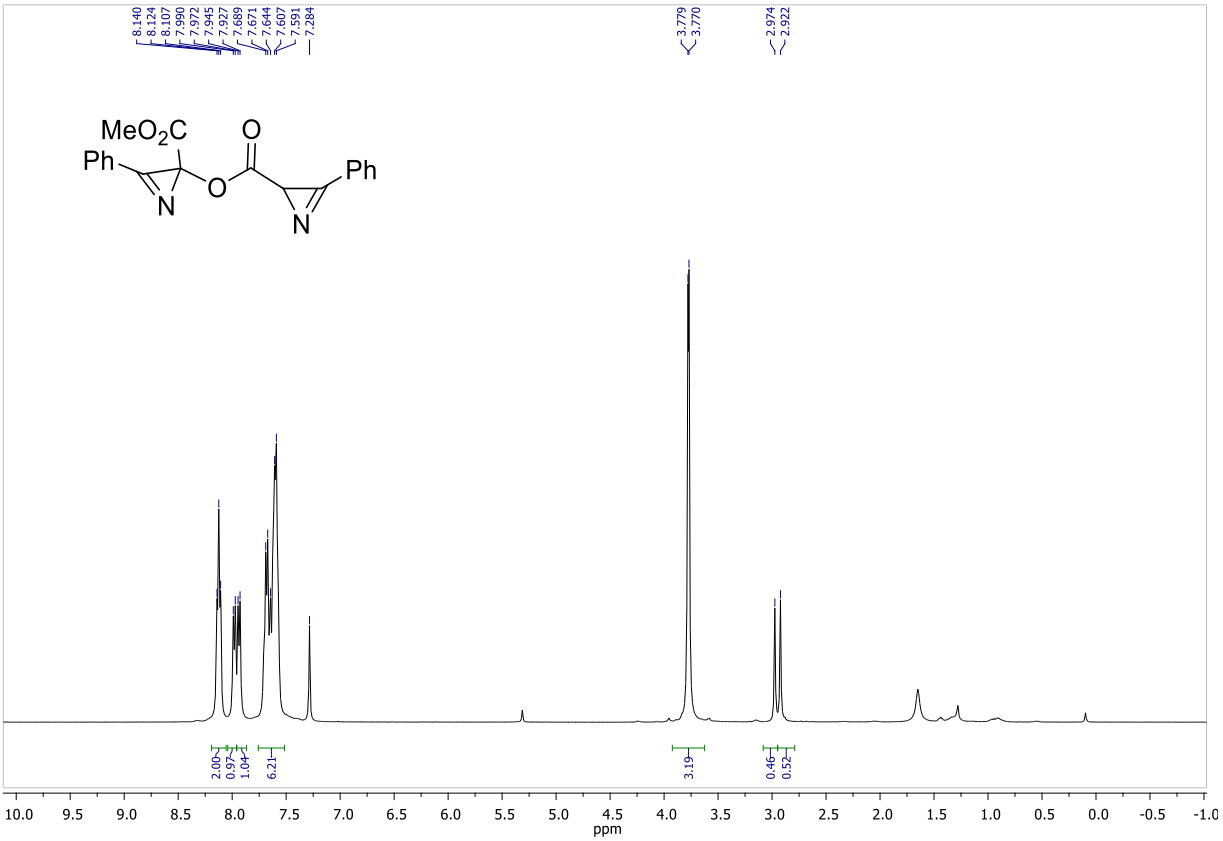


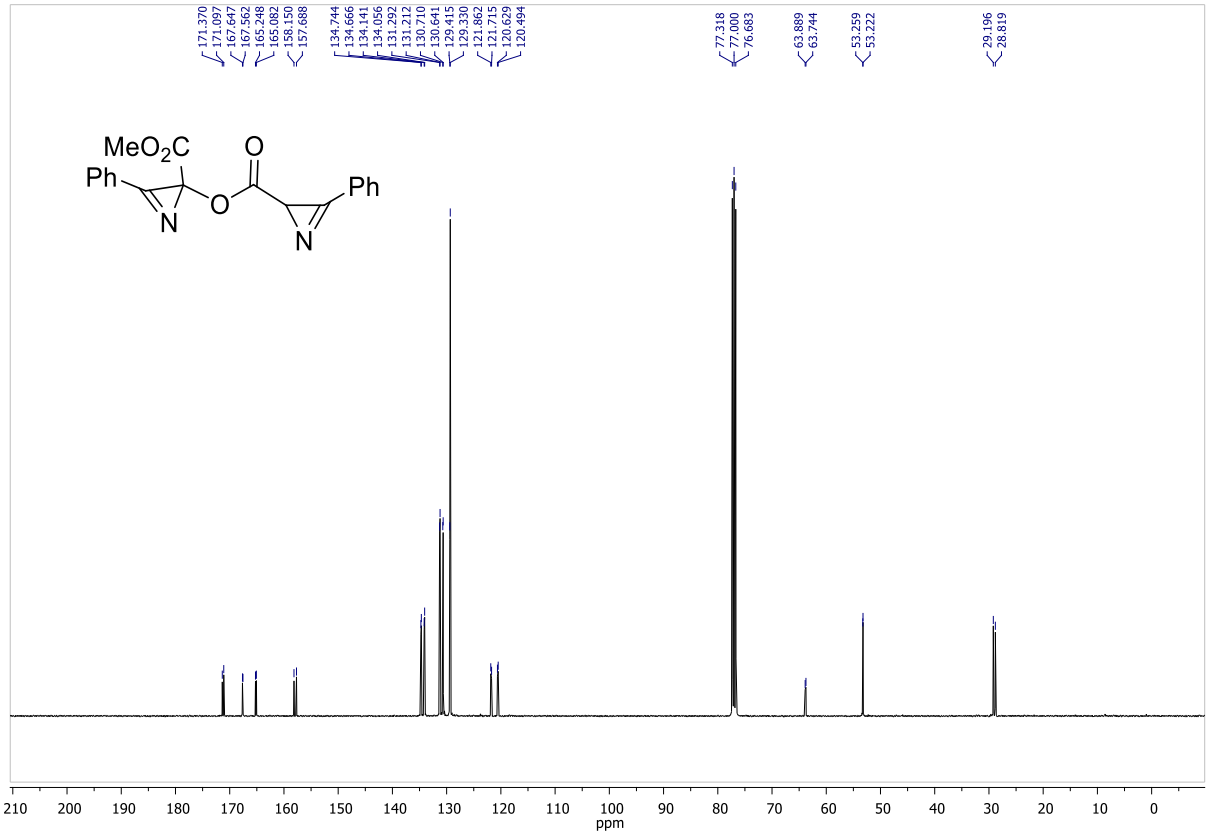
3-Phenyl-2*H*-azirine-2-carboxylic acid (**4**)



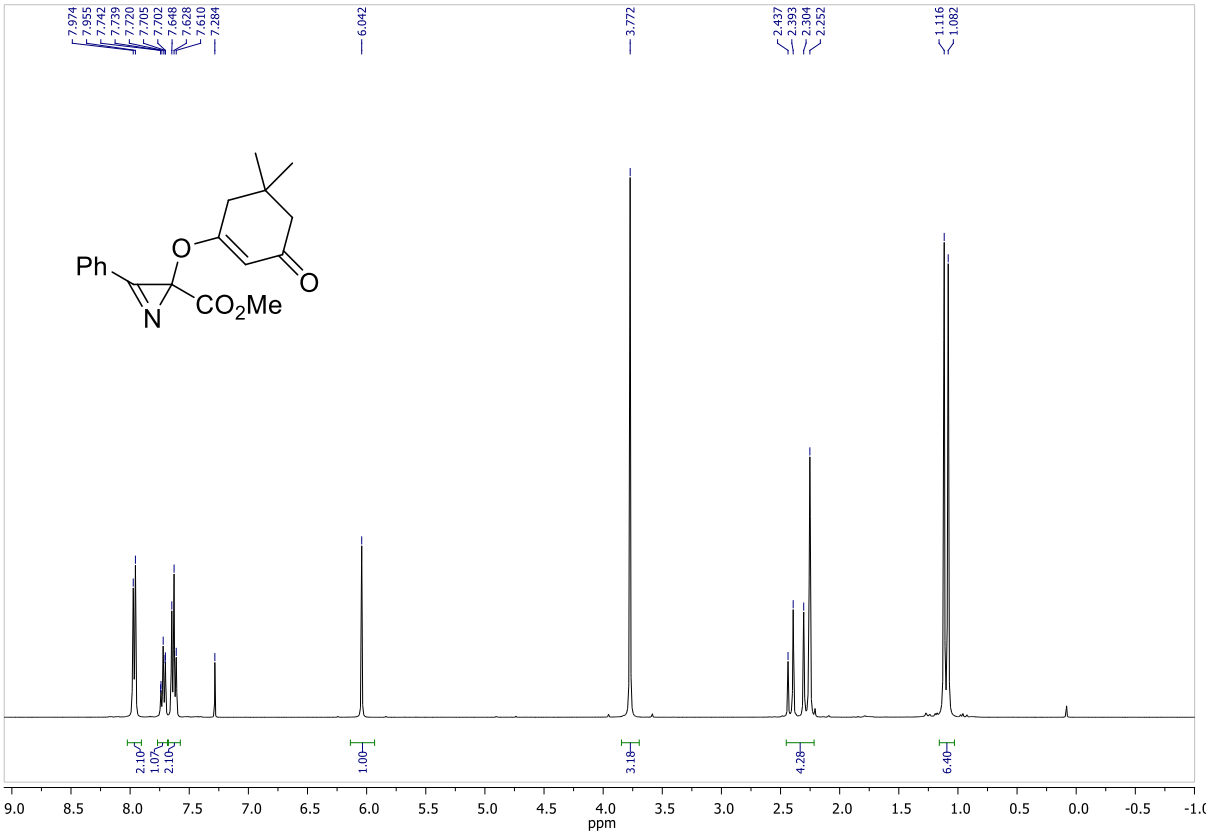


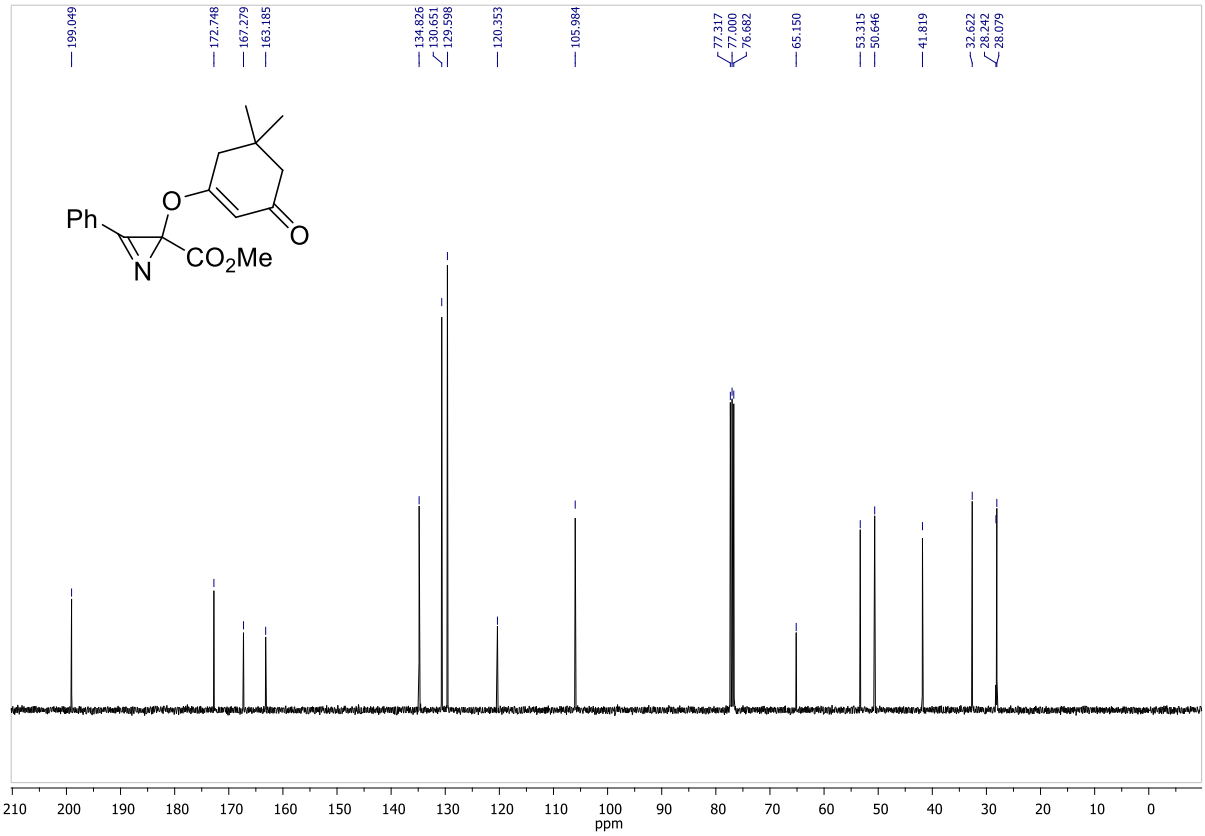
Methyl 3-phenyl-2-(3-phenyl-2*H*-azirine-2-carbonyloxy)-2*H*-azirine-2-carboxylate (**5**)

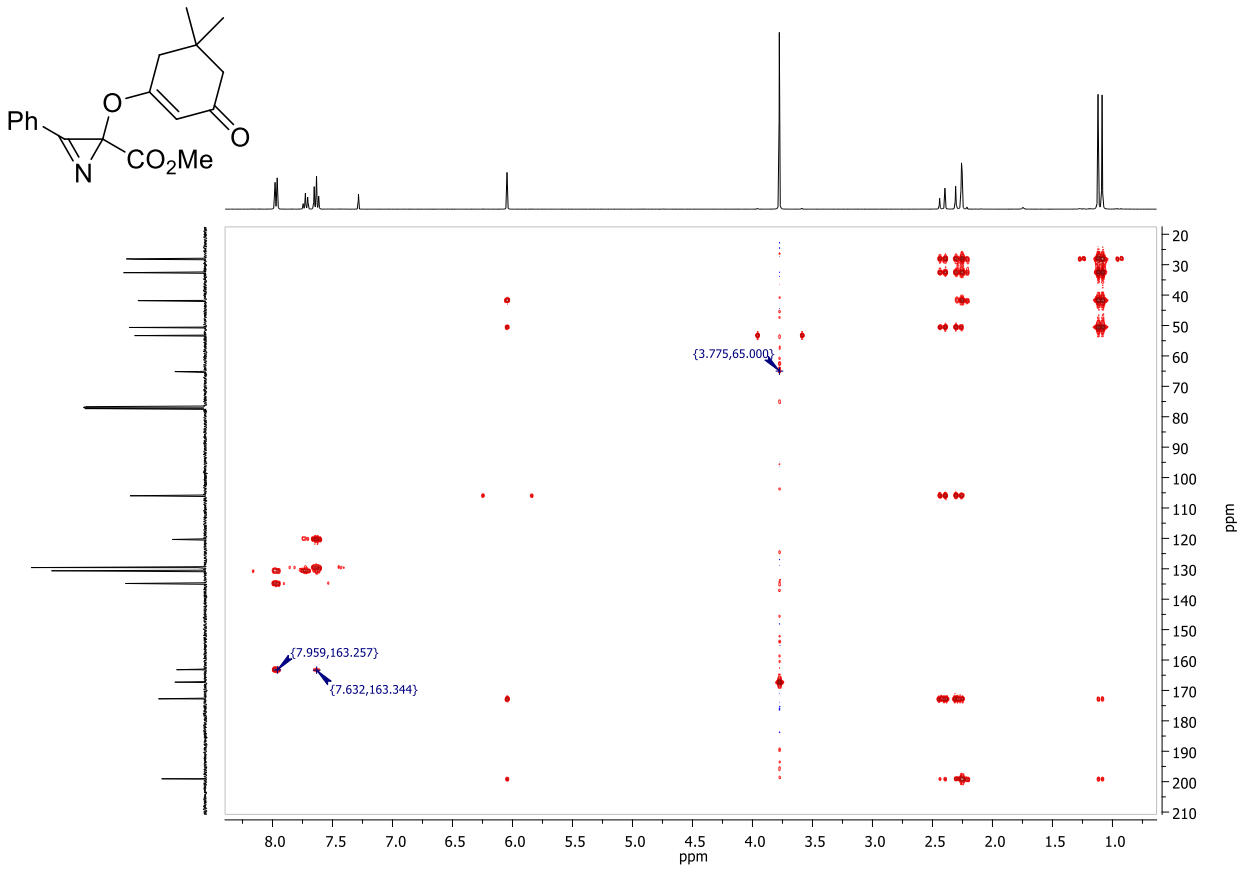




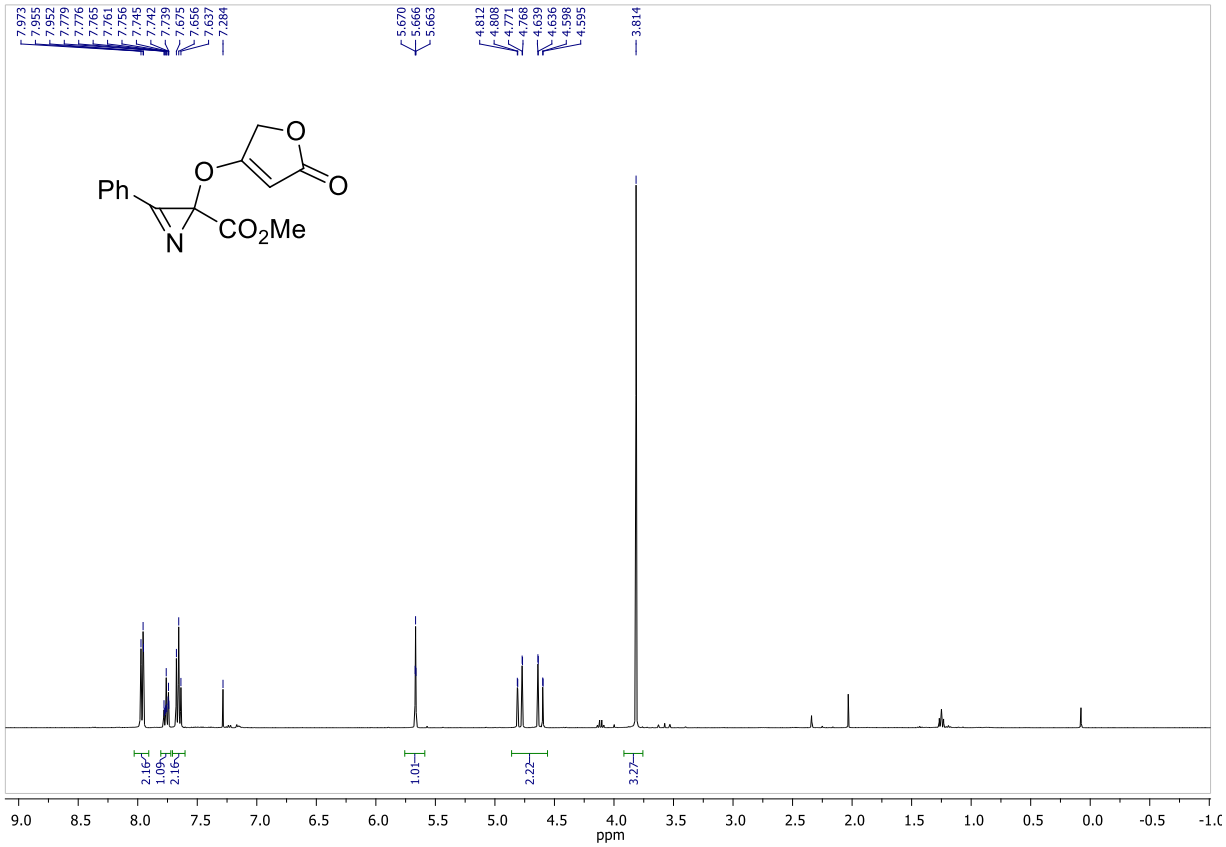
Methyl 2-(5,5-dimethyl-3-oxocyclohex-1-en-1-yloxy)-3-phenyl-2*H*-azirine-2-carboxylate (**7a**)

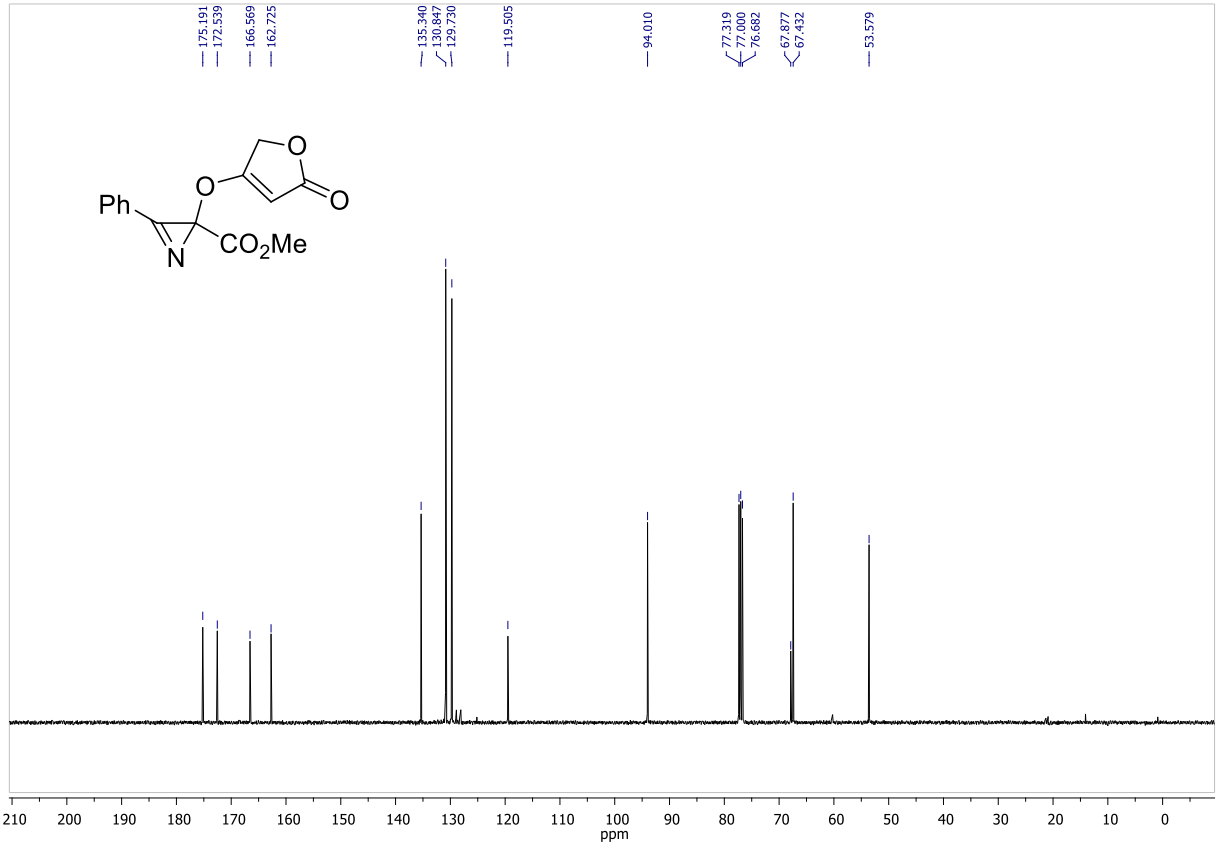




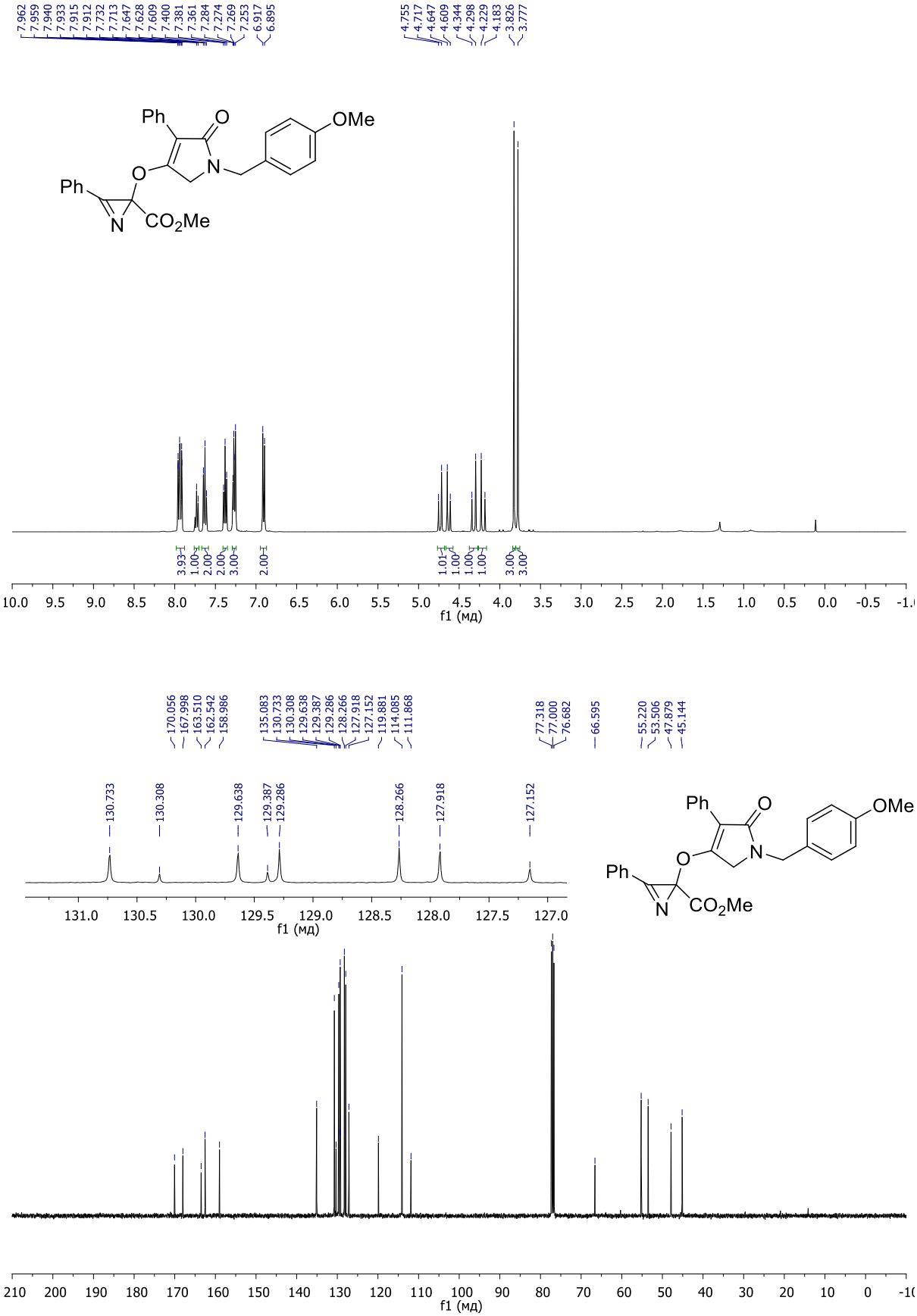

Ph
O
O
N
CO2Me
{3.775,65.000}
{7.959,163.257}
{7.632,163.344}
ppm
ppm

Methyl 2-(5-oxo-2,5-dihydrofuran-3-yloxy)-3-phenyl-2*H*-azirine-2-carboxylate (**7b**)

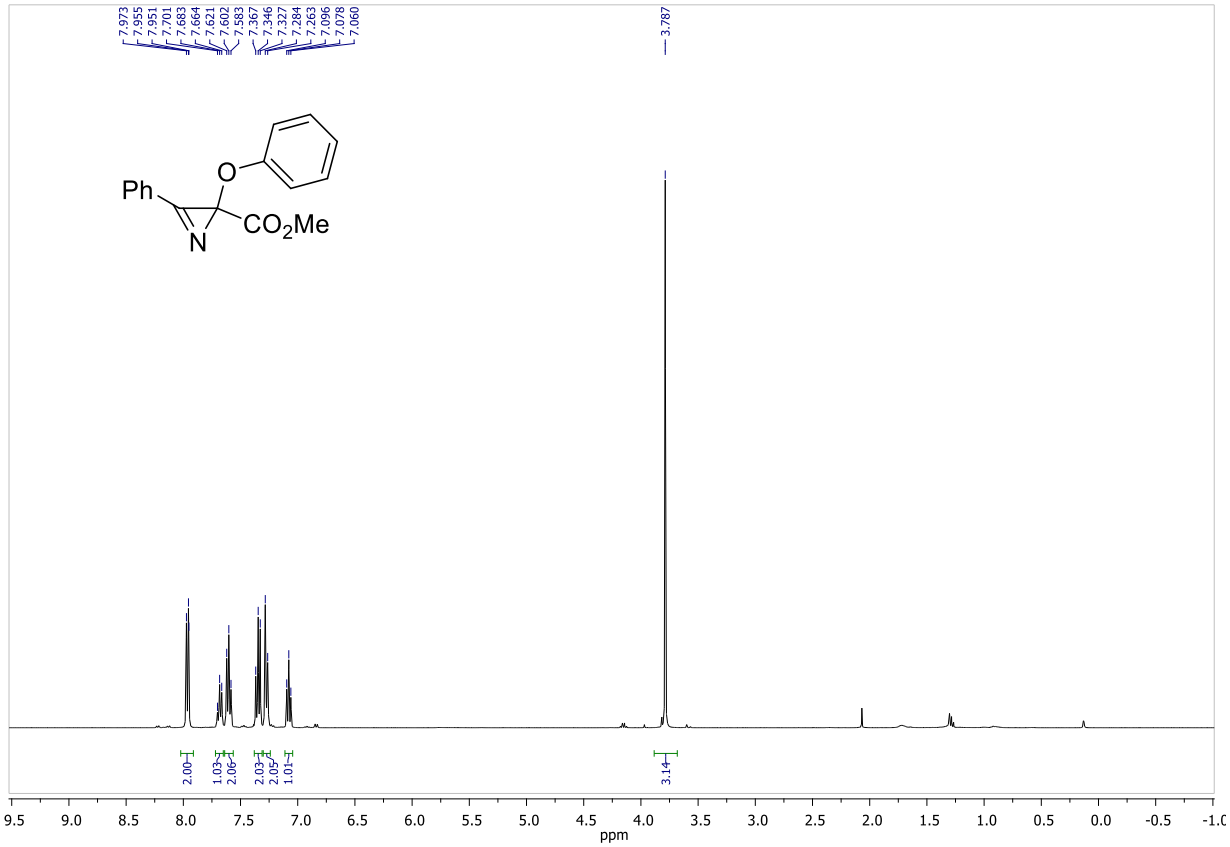


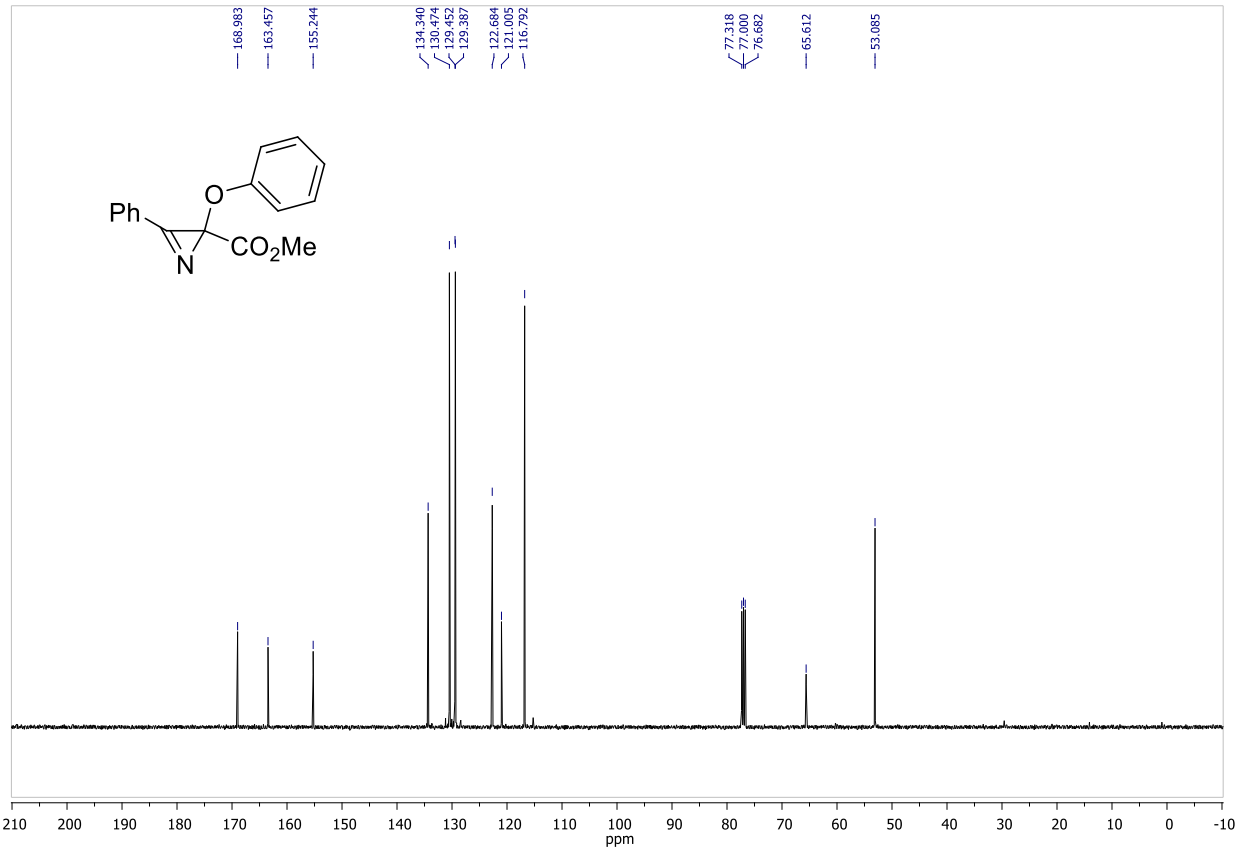


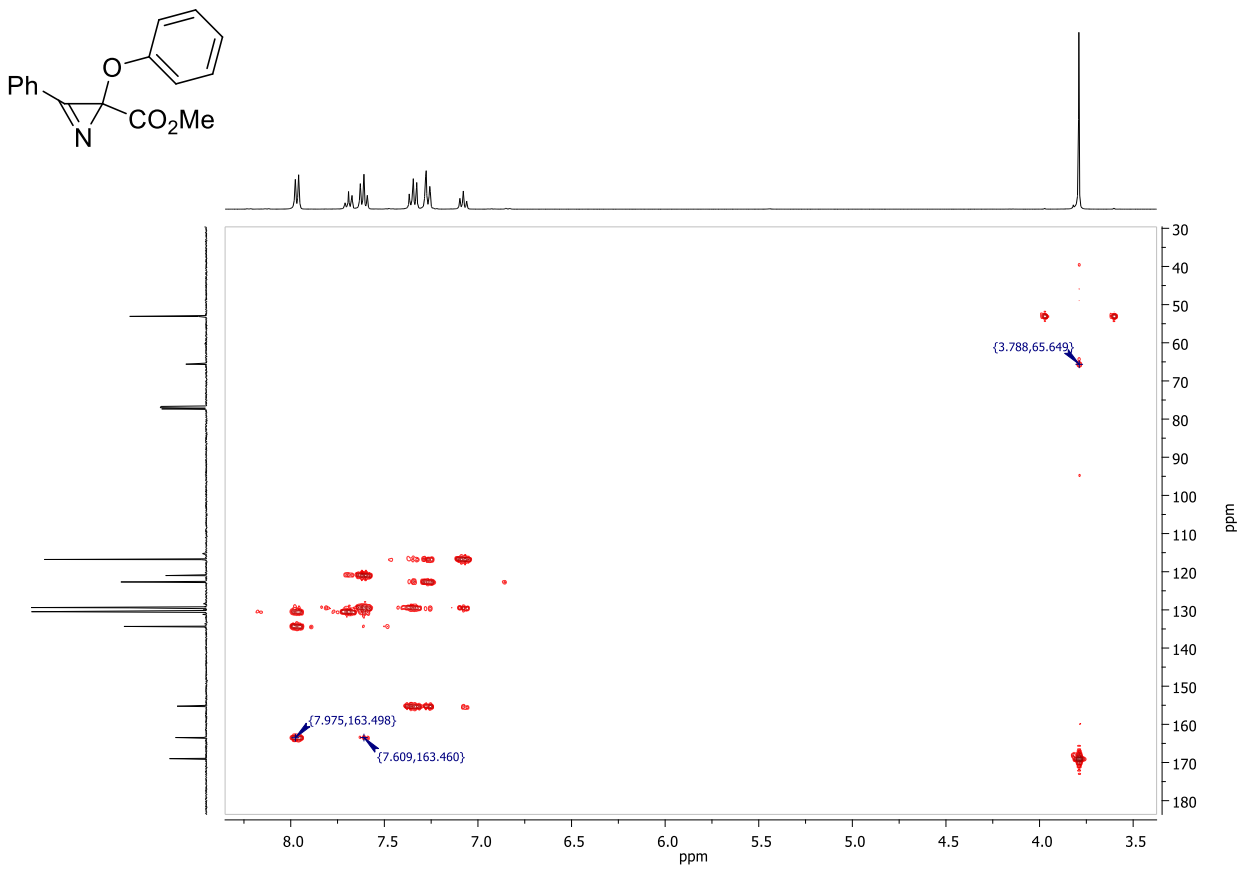
Methyl 2-[1-(4-methoxybenzyl)-5-oxo-4-phenyl-2,5-dihydro-1*H*-pyrrol-3-yloxy]-3-phenyl-2*H*-azirine-2-carboxylate (**7c**)



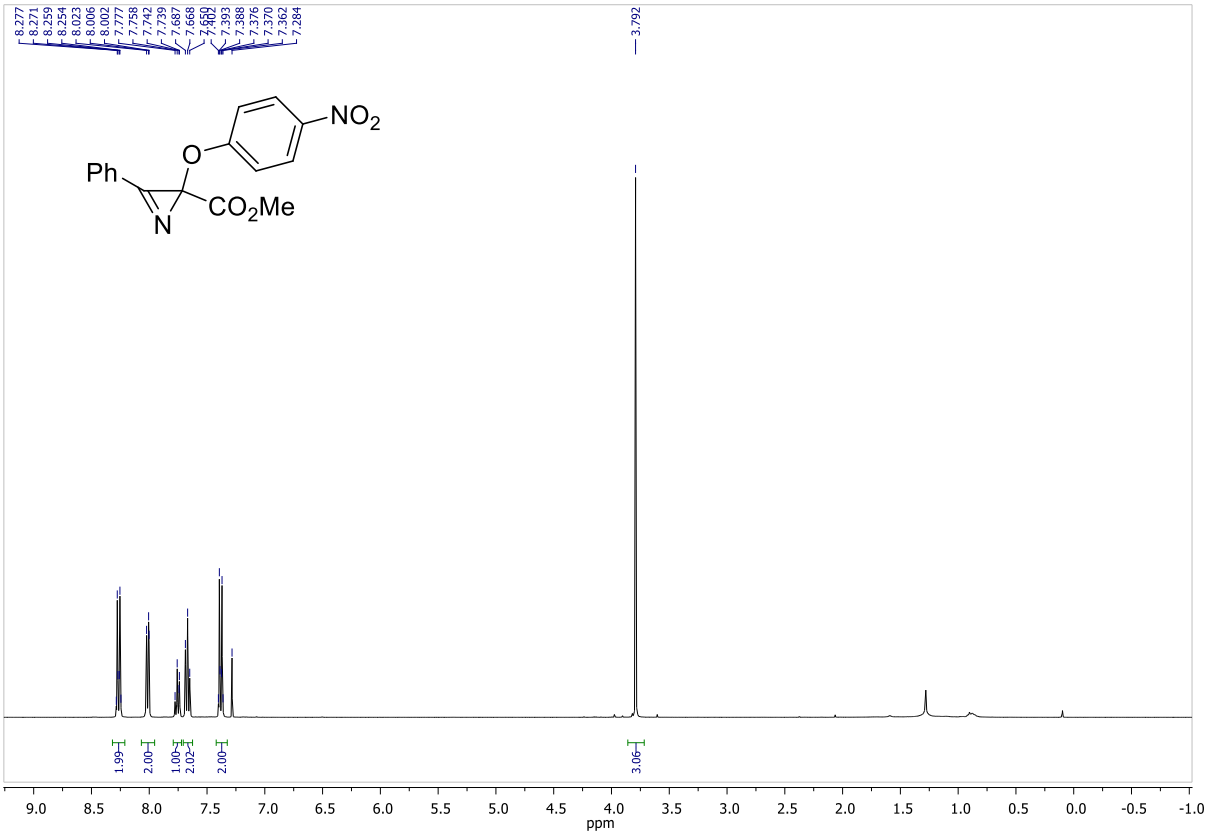
Methyl 2-phenoxy-3-phenyl-2*H*-azirine-2-carboxylate (**7d**)

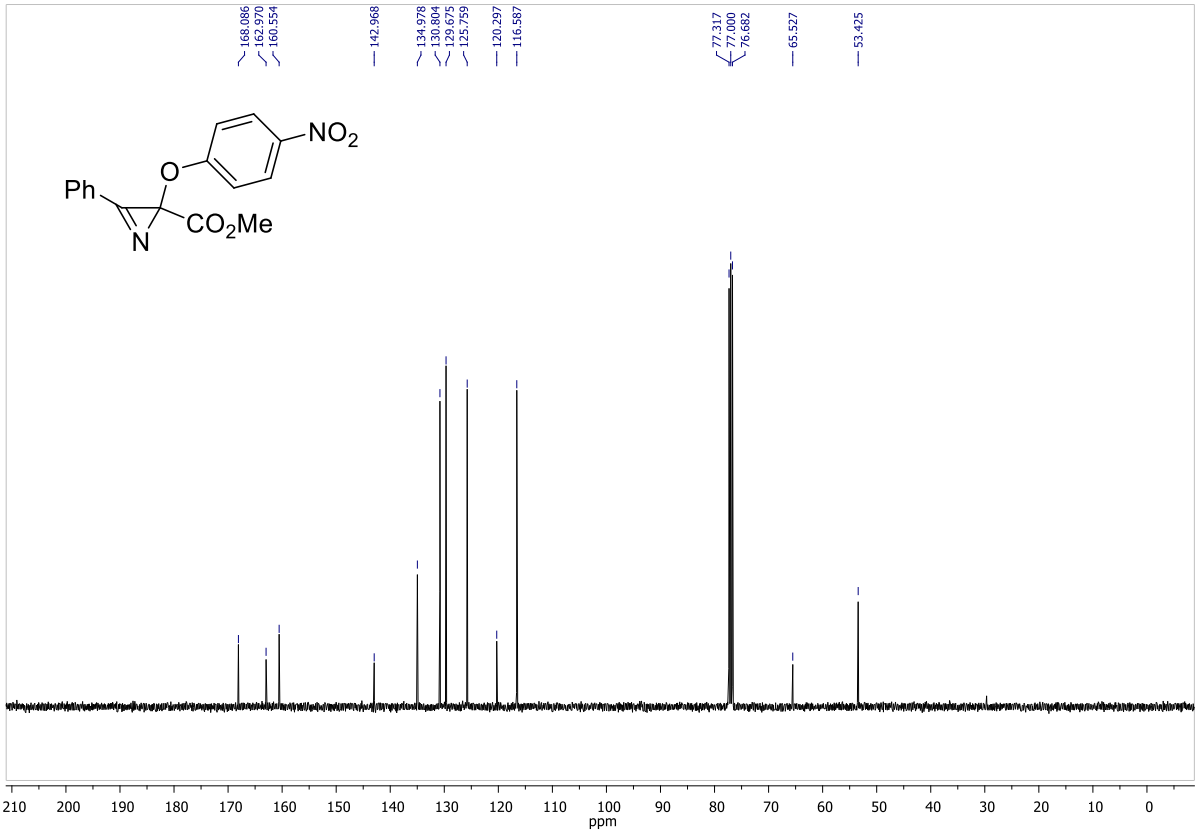




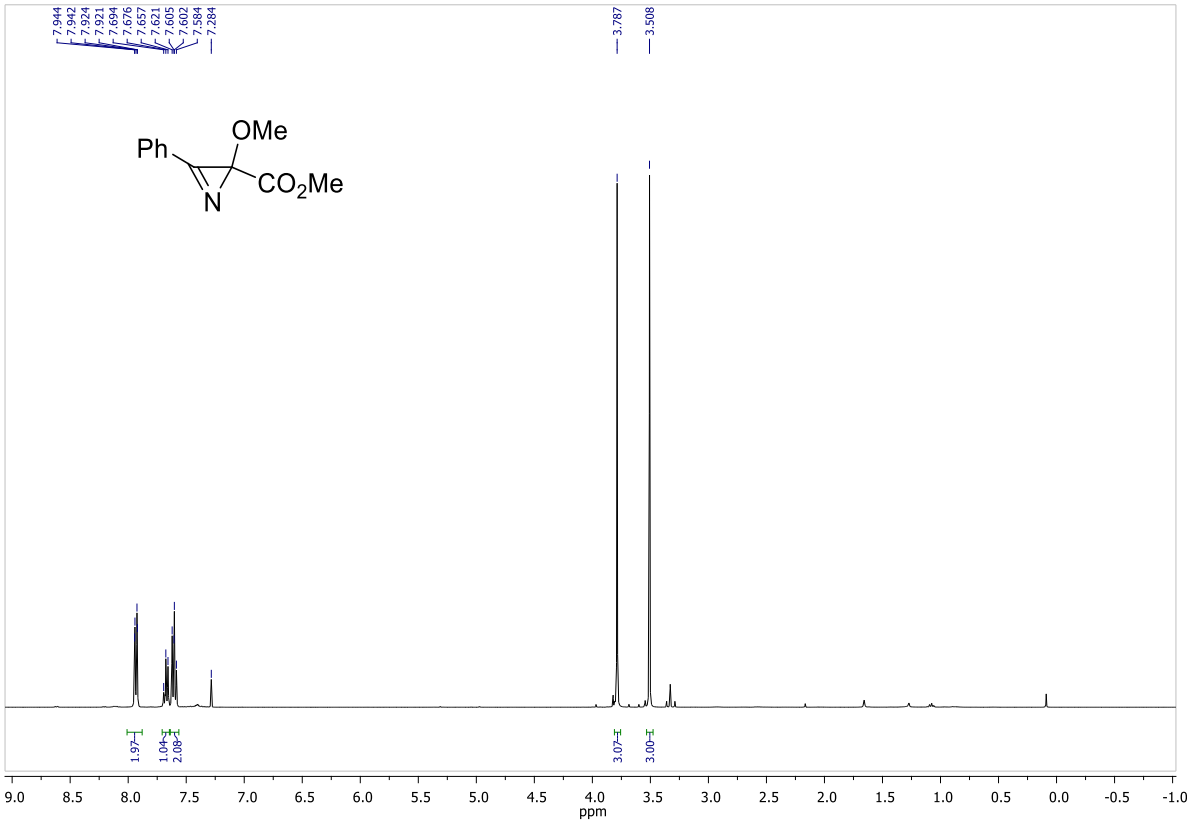

Ph
O
N
CO2Me
{3.788,65.649}
{7.975,163.498}
{7.609,163.460}
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
ppm
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
ppm

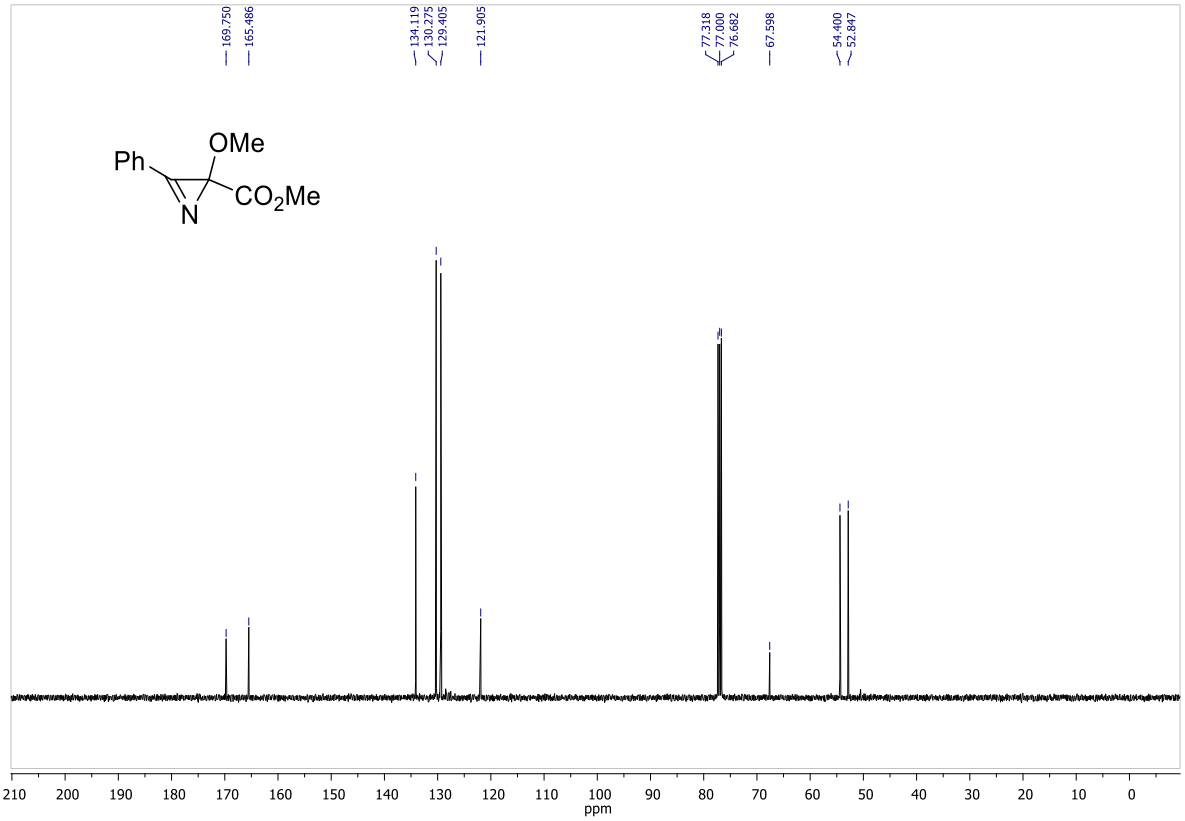
Methyl 2-(4-nitrophenoxy)-3-phenyl-2*H*-azirine-2-carboxylate (**7e**)





Methyl 2-methoxy-3-phenyl-2*H*-azirine-2-carboxylate (**7f**)





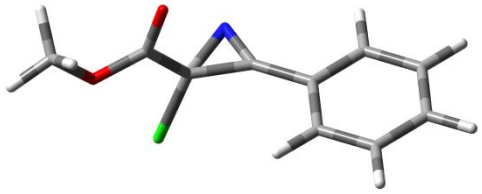
4. Calculation details

All calculations were performed by using the Gaussian 09 suite of quantum chemical programs.[1] Geometry optimizations of stationary points and transition states were performed at the DFT B3LYP using LANL2DZ basis set for chlorine atom and 6-31+G(d,p) basis set for all other atoms and PCM model for toluene. Stationary points on the respective potential-energy surfaces were characterized at the same level of theory by evaluating the corresponding Hessian indices. Careful verification of the unique imaginary frequencies for transition states was carried out to check whether the frequency indeed pertains to the desired reaction coordinate.

5. Table S-3. Energies (au) and Cartesian coordinates of stationary points of compounds **1c**, **2b**, **8a**, AcO^-, Cl^- and transition states TS^{S_N2}, $TS1^{syn}$, $TS1^{anti}$, $TS2^{syn}$, $TS2^{anti}$ and $TS2^{intr}$

Azirine **1c**

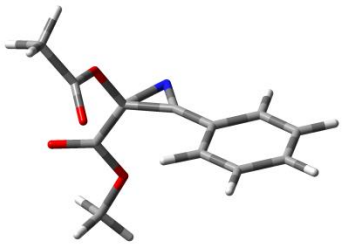
E_0 = -605.842515, E (298K) = -605.829529,
H (298K) = -605.828585, G (298K) = -605.884502.
Imaginary frequency = 0.



C	0.26730577	-0.55890191	-0.27598987
N	-0.42552323	-1.04337191	-1.22912687
C	-1.13008223	-0.69495491	0.03245913
C	1.60413777	-0.20222491	0.13050513
C	-2.07430323	0.48204209	-0.00057587
O	-3.19205023	0.30906509	0.70158513
Cl	-1.66737223	-2.12635191	1.08008713
O	-1.79358523	1.48452709	-0.63083387
C	-4.12593423	1.41368409	0.68887013
C	1.82647977	0.33068409	1.41178713
C	3.12019177	0.67706209	1.79926713
C	4.18703577	0.49313109	0.91281213
C	3.96617977	-0.03853991	-0.36480987
C	2.67814677	-0.39000891	-0.75995087
H	-4.95643323	1.09049709	1.31419313
H	-4.46035523	1.60881909	-0.33201387
H	-3.65387223	2.30863309	1.09952913
H	0.98983477	0.46726609	2.08991913
H	3.29738277	1.08826609	2.78805113
H	5.19380377	0.76427909	1.21686313
H	4.79863777	-0.17843191	-1.04734287
H	2.49265077	-0.80351891	-1.74639187

Azirine **2b**

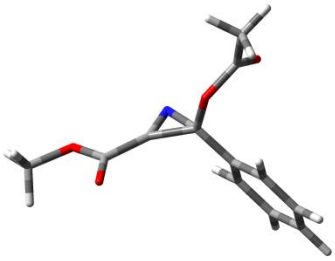
E_0 = -819.353224, E (298K) = -819.336943,
H (298K) = -819.335998, G (298K) = -819.399123.
Imaginary frequency = 0.



C	-0.15050889	0.20579634	0.56616992
N	-0.80064289	0.55580434	1.60108992
C	-1.58399189	0.10198534	0.40472792
C	1.18566511	0.03808034	0.04100492
C	-2.44098089	1.10179934	-0.32752708
O	-1.78430489	2.25670734	-0.51168808
O	-3.57836989	0.88464334	-0.69322008
C	-2.51854089	3.30592234	-1.18142608
C	1.36963111	-0.45436266	-1.26208808
C	2.66269911	-0.60328666	-1.76359808
C	3.76436811	-0.26274666	-0.97217608
C	3.58040711	0.22646734	0.32803792
C	2.29437011	0.37723734	0.83926092
H	-1.82906189	4.14665834	-1.23777708
H	-3.40593389	3.57098234	-0.60309108
H	-2.81428389	2.97851634	-2.18019408
H	0.50099511	-0.72346166	-1.85423108
H	2.81116111	-0.98499166	-2.76882608
H	4.76951411	-0.37899966	-1.36673508
H	4.43964211	0.48823034	0.93764192
H	2.13710411	0.75623334	1.84432292
C	-3.15033489	-3.18092666	-0.17611608
C	-2.31610689	-1.97141366	-0.49157008
O	-2.23839289	-1.13905966	0.58808292
O	-1.77403089	-1.73286466	-1.55085208
H	-3.05205689	-3.91237366	-0.97771408
H	-2.84891989	-3.61643766	0.78007392
H	-4.19812089	-2.87619666	-0.08536808

Azirine **8a**

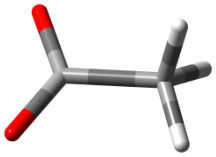
E_0 = -819.333183, E (298K) = -819.316611,
H (298K) = -819.315667, G (298K) = -819.380748.
Imaginary frequency = 0.



C	0.58850539	0.11632903	-0.03793541
N	-0.32638861	0.15274803	-1.25535541
C	-0.81928561	-0.16463697	-0.13381141
C	1.64891639	-0.93372797	0.07136759
C	-2.11103061	-0.56628697	0.49082059
O	-3.07821461	-0.63869497	-0.42397641
O	-2.22561661	-0.78784897	1.67814859
C	-4.39102361	-1.01863597	0.05959559
C	2.56232539	-0.90978897	1.13466059
C	3.53219539	-1.90740097	1.25085059
C	3.60060239	-2.93672297	0.30766659
C	2.69076839	-2.96340197	-0.75314041
C	1.71684939	-1.96974697	-0.86999341
H	-5.02886061	-1.01719697	-0.82192741
H	-4.73990861	-0.29223897	0.79594259
H	-4.34786461	-2.01233397	0.50941959
H	2.51326139	-0.11461397	1.87148059
H	4.23368239	-1.87952697	2.07948259
H	4.35642239	-3.71120297	0.39823759
H	2.74003239	-3.75546497	-1.49449441
H	1.01825039	-1.99042297	-1.70063341
C	2.03309939	3.45749003	0.60821959
C	1.82390039	2.16455803	-0.13278641
O	0.90557039	1.37933503	0.52458759
O	2.36262839	1.83282803	-1.16261141
H	2.77270639	4.06090803	0.08308459
H	1.08734039	4.00339603	0.67783859
H	2.37082339	3.25485603	1.62903859

Acetate-anion

E_0 = -228.554570, E (298K) = -228.550181,
H (298K) = -228.549237, G (298K) = -228.581822.
Charge = -1. Imaginary frequency = 0.



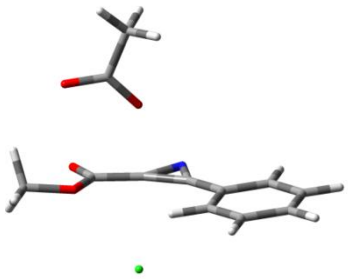
C	0.83856488	-0.06093368	0.12098593
C	-0.71120512	-0.01860268	0.11643593
O	-1.22905812	1.13571032	0.12585093
O	-1.31675112	-1.12872268	0.12590193
H	1.22142388	-1.05422068	-0.13197207
H	1.24196588	0.68196132	-0.57566507
H	1.19968588	0.20583432	1.12250393

Chloride-anion

E_0 = -15.068239, E (298K) = -15.066823,
H (298K) = -15.065879, G (298K) = -15.083262.
Charge = -1. Imaginary frequency = 0.

TS^{S_N2}

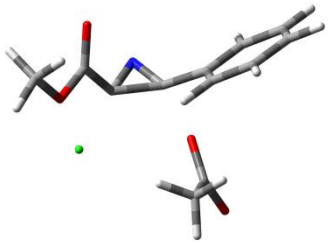
E_0 = -834.378594, E (298K) = -834.359630,
H (298K) = -834.358686, G (298K) = -834.428871.
Charge = -1. Imaginary frequency = 1.



C	0.79278648	-1.29661546	-0.13808843
N	0.14766348	-1.46917546	-1.28344743
C	-0.52528252	-1.65106046	-0.11398643
C	2.05951548	-0.94581346	0.42536457
C	-1.88381252	-2.00418346	0.38143757
O	-1.93926152	-1.94637146	1.70798257
Cl	0.11904648	-4.21521746	0.49101657
O	-2.79030052	-2.27892146	-0.37728243
C	-3.24720452	-2.14489746	2.27738957
C	2.21307348	-0.94740946	1.82324557
C	3.44302548	-0.59760746	2.37491957
C	4.51314448	-0.25808646	1.53796457
C	4.36079748	-0.26279346	0.14498857
C	3.13412248	-0.60596146	-0.41702943
H	-3.09363252	-2.12978046	3.35633857
H	-3.65290552	-3.10844346	1.96001857
H	-3.89292752	-1.32164746	1.96476557
H	1.37196048	-1.22291346	2.45024557
H	3.57188048	-0.59443746	3.45272757
H	5.47182648	0.01085354	1.97273057
H	5.19697748	0.00031254	-0.49547043
H	2.99524248	-0.61468046	-1.49347443
C	-1.83977552	2.79286654	0.38238357
C	-2.04555652	1.28094854	0.58559757
O	-1.11237352	0.54929454	0.09102957
O	-3.07241852	0.88609454	1.17761457
H	-2.57336752	3.36429354	0.95633557
H	-0.82614252	3.08544454	0.67534157
H	-1.95292452	3.03155754	-0.68149843

$TS1^{syn}$

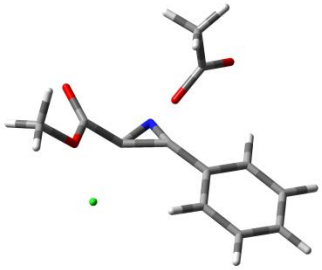
E_0 = -834.380145, E (298K) = -834.362345,
H (298K) = -834.361401, G (298K) = -834.428182.
Charge = -1. Imaginary frequency = 1.



C	-0.72192099	-0.89398066	-1.52045583
N	-0.02262199	-0.92747966	-2.63346383
C	0.72141801	-0.86597566	-1.42843283
C	-1.86643199	-1.68396266	-1.03561183
C	1.56487401	-2.04636966	-1.00873183
O	2.38509301	-1.80906766	0.02820017
Cl	1.64750801	0.79116134	-1.01660583
O	1.45665501	-3.13765266	-1.53878483
C	3.16261401	-2.93305666	0.48052017
C	-1.83904199	-2.29364966	0.22540117
C	-2.90728399	-3.09219966	0.64501817
C	-4.01083299	-3.28238066	-0.19086683
C	-4.03922799	-2.67566266	-1.45328383
C	-2.97234999	-1.88398266	-1.87672683
H	3.77503601	-2.54930266	1.29620617
H	3.79188401	-3.31150866	-0.32866983
H	2.50775601	-3.73426066	0.83331817
H	-0.98308499	-2.14364566	0.87649517
H	-2.87615799	-3.56247366	1.62415317
H	-4.84322899	-3.89950266	0.13641517
H	-4.89472899	-2.82071366	-2.10730483
H	-2.98801399	-1.41005466	-2.85271983
C	-1.33227299	1.04217334	1.10419517
C	-1.78410999	1.58455234	-0.25294283
O	-1.53593899	0.87884134	-1.31008783
O	-2.39417499	2.67059134	-0.29219083
H	-1.31774599	1.85190734	1.83670217
H	-2.04629499	0.28223034	1.44201117
H	-0.34426299	0.58018634	1.04340817

TS1^{anti}

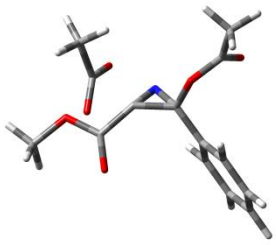
E_0 = -834.391100, E (298K) = -834.372826,
H (298K) = -834.371882, G (298K) = -834.439847.
Charge = -1. Imaginary frequency = 1.



C	0.44181398	-0.57517254	-0.45104969
N	-0.16585002	-0.57751654	-1.63267969
C	-0.85907202	-1.12210054	-0.55438269
C	1.78112398	-0.84610054	0.07080031
C	-2.19372802	-0.65732454	-0.03371869
O	-2.36751802	-0.97314654	1.25840431
Cl	-1.03614502	-3.16360754	-0.55033769
O	-3.00753102	-0.05867754	-0.70816169
C	-3.61158702	-0.55249854	1.84571231
C	1.92746398	-1.49785754	1.30374831
C	3.20159098	-1.80776454	1.78300731
C	4.33348098	-1.46812854	1.03376731
C	4.18691298	-0.81720154	-0.19723069
C	2.91537198	-0.50720754	-0.68121169
H	-3.57124502	-0.89030354	2.88103531
H	-4.45466102	-1.01311754	1.32389931
H	-3.70386602	0.53537846	1.79964331
H	1.04214298	-1.75962954	1.87422431
H	3.31115698	-2.31540554	2.73751531
H	5.32551398	-1.70844354	1.40737831
H	5.06485398	-0.54797654	-0.77816869
H	2.78898598	0.01574046	-1.62255869
C	-0.05419902	3.51567646	0.74070631
C	0.52928198	2.25365546	0.08887131
O	0.06902198	1.15049946	0.57841231
O	1.35505998	2.36211546	-0.83650369
H	0.50772598	4.40184646	0.43578031
H	-1.09792102	3.62939346	0.42501931
H	-0.04889602	3.42557446	1.83161631

TS2^{syn}

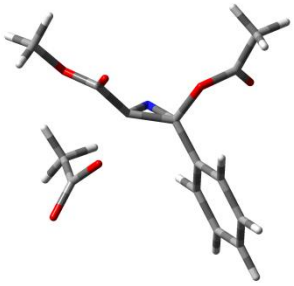
E_0 = -1047.888256, E (298K) = -1047.867044,
H (298K) = -1047.866100, G (298K) = -1047.941501.
Charge = -1. Imaginary frequency = 1.



C	0.89670160	0.53828021	-0.49678748
N	0.29502860	0.19218521	-1.77972648
C	-0.38642340	-0.10637079	-0.70389048
C	2.15199560	-0.13362379	-0.02251548
C	-1.05529540	-1.37477879	-0.29007248
O	-2.20659140	-1.59197679	-0.94557748
O	-0.54283340	-2.17229479	0.47216452
C	-2.88934740	-2.81457179	-0.61544948
C	2.75855560	0.22550821	1.19020352
C	3.91869660	-0.42054779	1.62346352
C	4.49262460	-1.43411579	0.84974152
C	3.89152760	-1.79700779	-0.35973348
C	2.72837060	-1.15517079	-0.78920848
H	-3.79835540	-2.80858879	-1.21688848
H	-3.13267140	-2.83253879	0.44946352
H	-2.27094140	-3.68111079	-0.86413748
H	2.31536160	1.00853521	1.79699352
H	4.37238260	-0.13341979	2.56858752
H	5.39539260	-1.93675579	1.18651852
H	4.32893260	-2.58205379	-0.97125948
H	2.25664260	-1.43426179	-1.72586848
C	1.25197160	4.22735421	-0.17394548
C	1.56495660	2.83936521	-0.68642848
O	0.81590960	1.92047121	-0.04908848
O	2.37951060	2.59475821	-1.55764848
H	1.94884260	4.94552121	-0.60686348
H	0.22739660	4.49121921	-0.45465048
H	1.30957760	4.25436421	0.91802552
C	-3.47844840	2.33100921	0.89851852
C	-2.48326440	1.17442221	0.73946952
O	-1.85784240	1.16867821	-0.38660448
O	-2.33240040	0.35644221	1.66776752
H	-4.17469240	2.12651221	1.71541352
H	-2.92333840	3.24735221	1.13111452
H	-4.02619740	2.50475621	-0.03232248

TS2^{anti}

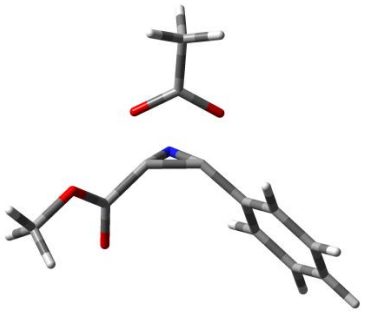
E_0 = -1047.886947, E (298K) = -1047.865891,
H (298K) = -1047.864947, G (298K) = -1047.939431.
Charge = -1. Imaginary frequency = 1.



C	-0.62537855	0.80594145	0.37447280
N	0.27830645	0.69952045	1.49943780
C	0.79427245	0.53316345	0.28860880
C	-1.73030555	-0.16923155	0.09183580
C	1.94840345	1.19502745	-0.39647020
O	3.07499845	1.10906645	0.34322580
O	1.89203945	1.76904745	-1.46727320
C	4.25358845	1.69975545	-0.23366420
C	-2.00064755	-1.19821555	1.00050480
C	-3.01702255	-2.12202955	0.74803180
C	-3.77696655	-2.02986855	-0.42190020
C	-3.51048755	-1.00532155	-1.33596220
C	-2.49444655	-0.08129355	-1.08069520
H	5.04960745	1.52550545	0.49005080
H	4.10628245	2.77121745	-0.39056320
H	4.49056145	1.22244645	-1.18785620
H	-1.40687455	-1.26061055	1.90670880
H	-3.21440555	-2.91454555	1.46514980
H	-4.56525055	-2.75082655	-0.62181320
H	-4.08979355	-0.92924655	-2.25266020
H	-2.28670455	0.70851745	-1.79633120
C	-2.07054255	4.25529445	0.22649980
C	-1.87794155	2.84549045	0.74267980
O	-0.99858455	2.17411545	-0.02395120
O	-2.44405755	2.38780145	1.71836380
H	-2.81436555	4.77076045	0.83470380
H	-1.11961055	4.79585945	0.26502780
H	-2.39147555	4.23339345	-0.81947520
C	2.12762645	-1.83101555	1.71181780
C	1.69166345	-2.08842355	0.27637280
O	1.14491345	-1.10561955	-0.39896820
O	1.87402945	-3.19971155	-0.23913320
H	2.41367745	-2.77509155	2.17838080
H	2.98552245	-1.15007755	1.71120680
H	1.33813445	-1.33656855	2.28298380

TS^{intr}

E_0 = -819.306766, E (298K) = -819.291184,
H (298K) = -819.290239, G (298K) = -819.352255.
Charge = 0. Imaginary frequency = 1.



C	0.13799246	0.56597308	0.74465142
N	0.78974046	0.25409508	1.91582542
C	1.43574646	-0.05079892	0.76232742
C	-1.23248154	0.22278708	0.30044442
C	2.02895046	-1.34187892	0.29717242
O	3.13713546	-1.20783992	-0.43597958
O	1.49422746	-2.39847892	0.56983542
C	3.72347346	-2.44013892	-0.91674658
C	-1.73870554	0.63777108	-0.93980158
C	-3.02821454	0.26918308	-1.32526758
C	-3.81839954	-0.51586392	-0.47879758
C	-3.31482554	-0.93025192	0.75736842
C	-2.02597854	-0.56197092	1.14858542
H	4.60833346	-2.13536192	-1.47287758
H	3.01791046	-2.96409792	-1.56460758
H	3.99520846	-3.08026192	-0.07515658
H	-1.13008254	1.25388908	-1.59317058
H	-3.41611754	0.59389208	-2.28627358
H	-4.82120354	-0.80216792	-0.78214858
H	-3.92421854	-1.53896192	1.41864742
H	-1.62193654	-0.88421392	2.10265842
C	2.29565446	3.59019508	-0.14622658
C	1.71503946	2.23496208	0.10117042
O	0.44049946	2.11246408	0.22722042
O	2.47602146	1.22061308	0.21490042
H	3.23590146	3.50225508	-0.69240758
H	1.58381746	4.21445008	-0.68851858
H	2.49851646	4.05743808	0.82423942

6. Literature

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