

**Site-selective α -C-H Functionalization of Trialkylamines via
Reversible HAT-Catalysis**

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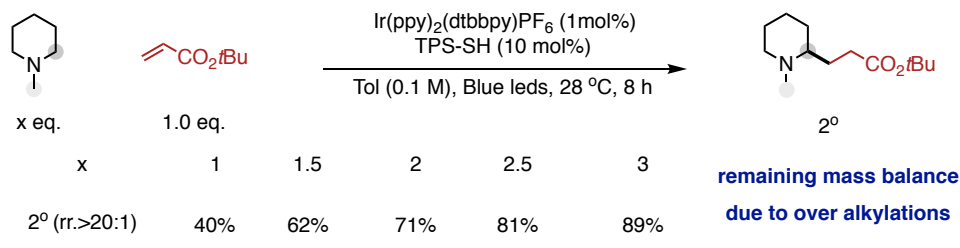
I. General consideration

Reagents: Unless otherwise noted, all reactions were carried out in reaction tubes with screw cap. Anhydrous solvents and reagents were purchased from Sigma Aldrich and used without further purification. All other reagents were purchased from commercial sources and used as received. For the pharmaceuticals received in salt form, a simple treatment with K_2CO_3 (aq.) and ethyl acetate offered pure enough sample for the reactions. Purification of the product was conducted either manually on SiliCycle® SilicaFlash® P60 (230-400 mesh) silica gel or automatically via a Teledyne Isco Lumen CombiFlash using CombiFlash gold pre-packed columns. Thin layer chromatography (TLC) was performed on Silicycle 250 μm silica gel 60 Å plates. Visualization was accomplished with UV lamp (254 nm), $KMnO_4$ or Iodine. A Kessil blue LED (34W maximum, 24 VDC, 440 nm) was used as the light source for the photoredox catalyzed reactions. The procedures described in this section are representative. Thus, the yields may differ slightly from those given in the tables of the manuscript.

Analytical Methods: 1H NMR, ^{13}C NMR and ^{19}F NMR spectra are included for all new compounds. 1H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded on Varian 300/400 MHz or Bruker 400/500 MHz at ambient temperature. All 1H NMR spectra are reported in parts per million (ppm) downfield of TMS and were measured relative to the signals for $CHCl_3$ (7.26 ppm). All ^{13}C NMR spectra were reported in ppm relative to residual $CHCl_3$ (77.16 ppm) and were obtained with 1H decoupling. Coupling constants, J , are reported in hertz (Hz). In the case of diastereoisomeric mixtures, isolated NMR was recorded to determine the ratio. High resolution mass spectra (HRMS) were obtained from the Columbia University Chemistry Department Mass Spectrometry Facility on a Waters XEVO G2XS QToF mass spectrometer equipped with a UPC2 SFC inlet and a LockSpray source with one of the following three probes: electrospray ionization (ESI) probe, atmospheric pressure chemical ionization (APCI) probe, or atmospheric pressure solids analysis probe (ASAP). Infrared spectra were collected on a Perkin Elmer Spectrum Two FT-IR Spectrometer. Infrared spectra were recorded on a Bruker Tensor 27. Mass spectra were recorded on a Waters LCT Premier spectrometer. Stern-Volmer luminescence quenching experiments were conducted on a Fluoromax-4 fluorometer.

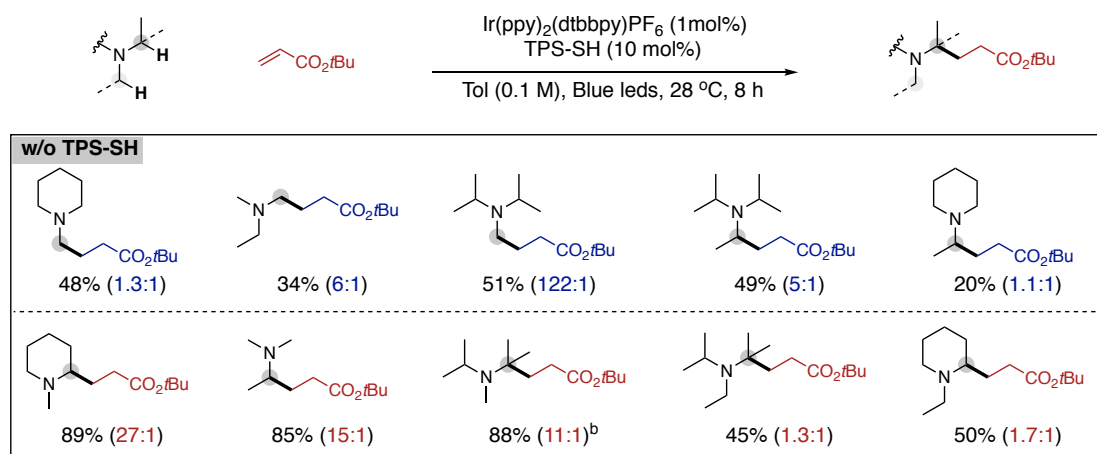
II. Optimization details and control experiments

Table S1. Practical considerations of amine loadings

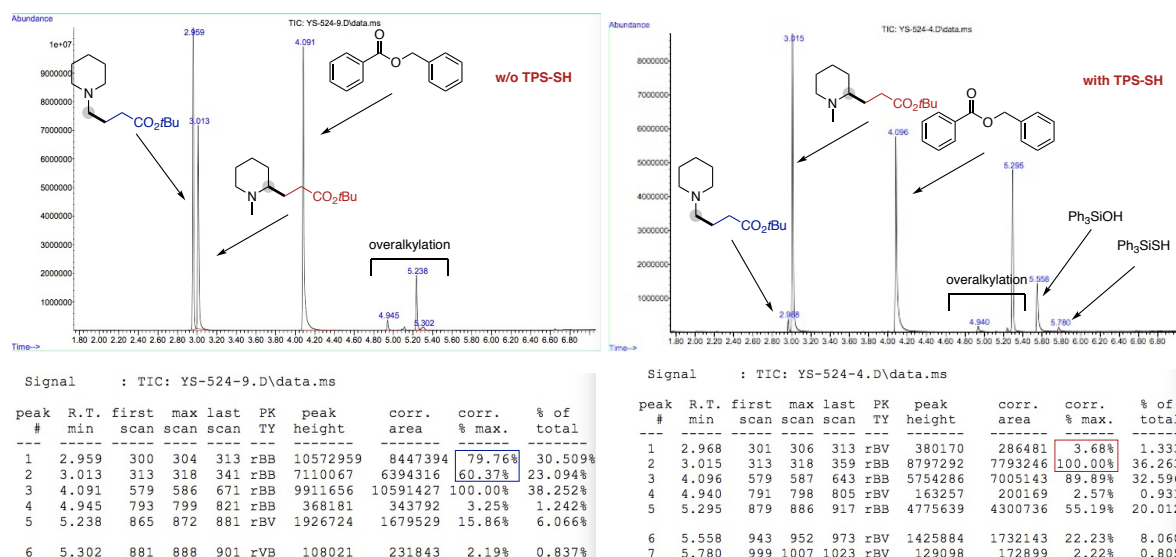


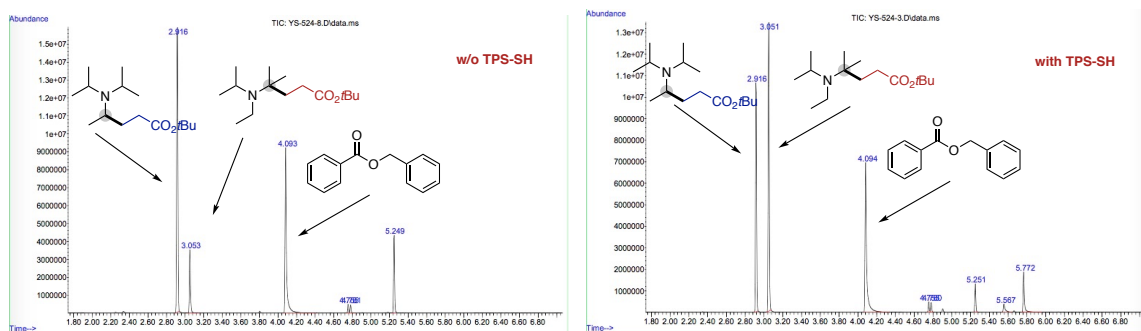
^a yield and ratio are determined by GC-MS analysis with benzyl benzoate as internal standard

Table S2. Control experiments with/without TPS-SH



^a yield and ratio are determined by GC-MS analysis with benzyl benzoate as internal standard; ^b *m*-Xylene was used





Signal : TIC: YS-524-8.D\data.ms

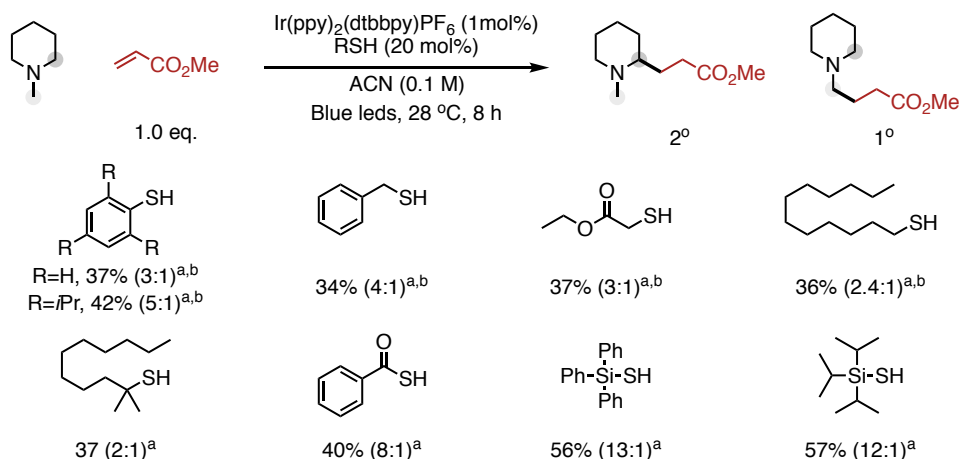
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.916	288	293	299	rBB	15889797	14654632	100.00%	46.279%
2	3.053	321	328	352	rBB	3528129	2919472	19.92%	9.220%
3	4.093	579	587	665	rBB	9225513	10008394	68.30%	31.606%
4	4.755	747	752	755	rBV	488596	369561	2.52%	1.167%
5	4.781	755	758	773	rVB	456804	365813	2.50%	1.155%
6	5.249	869	875	881	rBB	4315988	3348188	22.85%	10.573%

Signal : TIC: YS-524-3.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.916	289	293	299	rBB	10630106	8452810	76.82%	26.710%
2	3.051	322	327	333	rBB	13429119	11004059	100.00%	34.771%
3	4.094	579	587	645	rBB	6957237	8202036	74.54%	25.917%
4	4.755	747	752	755	rBV	486999	369866	3.36%	1.169%
5	4.780	755	758	763	rVB	450243	353539	3.21%	1.117%
6	5.251	870	875	881	rBB	1318309	946432	8.60%	2.991%
7	5.567	945	973	973	rBV	377775	568364	5.17%	1.796%
8	5.772	998	1005	1051	rBB	1864428	1749969	15.90%	5.530%

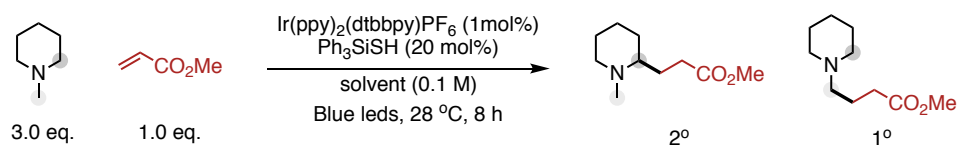
Note: Due to overlapping peaks in the spectra, $^1\text{H-NMR}$ analysis is unreliable as a method to determine the regioisomer ratios. We thus tentatively assign the ratios by GC-MS analysis, understanding that there are caveats with this method (efforts towards synthesis of minor isomer to correct the GC-MS results failed due to oligomer contamination). Notably, during the purification of the products, we only observe <5% or trace of minor isomers (mono-alkylation at the methyl position) when using more electron-deficient olefins (vinyl phenyl sulfone) as radical acceptor, unless otherwise noted.

Table S3. Optimization of thiol catalyst for *N*-Me piperidine



yield and ratio are determined by GC-MS analysis with benzyl benzoate as internal standard;
^a yield of 2° product, ratio of 2°:1°; ^b sulfa-Michael addition observed.

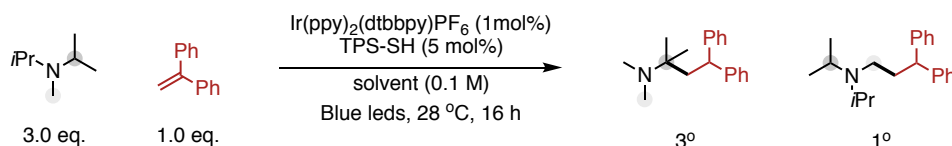
Table S4. Optimization of solvent for *N*-Me piperidine



solvent	2° : 1°	yield (2°) (%)	solvent	2° : 1°	yield (2°) (%)
ACN	13	56	DMF	13	77
Acetone	13	70	DMA	13	79
Tol	17	72	NMP	12	76
CF ₃ Ph	14	78	DMSO	12	72
DCM	14	63	DME	12	73
DCE	11	52	EtOAc	13	76

yield and ratio are determined by GC-MS analysis with benzyl benzoate as internal standard

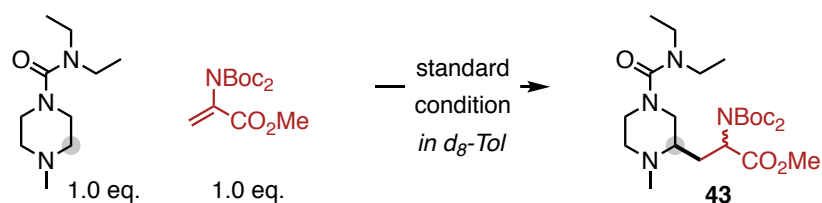
Table S5. Optimization of solvent for *N*, *N*-diisopropylmethylamine



solvent	3° : 1°	yield (3°) (%)	solvent	3° : 1°	yield (3°) (%)
ACN	0.7	23	EtOH	1	24
Tol	1.7	38	Et ₂ O	1.8	15
CF ₃ Ph	0.4	21	DME	1.3	41
DMF	0.7	18	THF	1.6	47
NMP	0.8	21	Dioxane	1.8	54^b
DMSO	0.5	12	Diglyme	0.5	11

^a yield and ratio are determined by GC-MS analysis with benzyl benzoate as internal standard
^b w/o TPS-SH, only 1° product (52% yield) observed.

Table S6. Practical consideration of alkylation of diethylcarbamazine



irradiation time (h)	conversion of olefin (%)	yield of 43 (%)
1	57	27
2	87	31
4	100	33

0.2 mmol scale. 0.1 mmol of ethyl benzoate as internal standard.

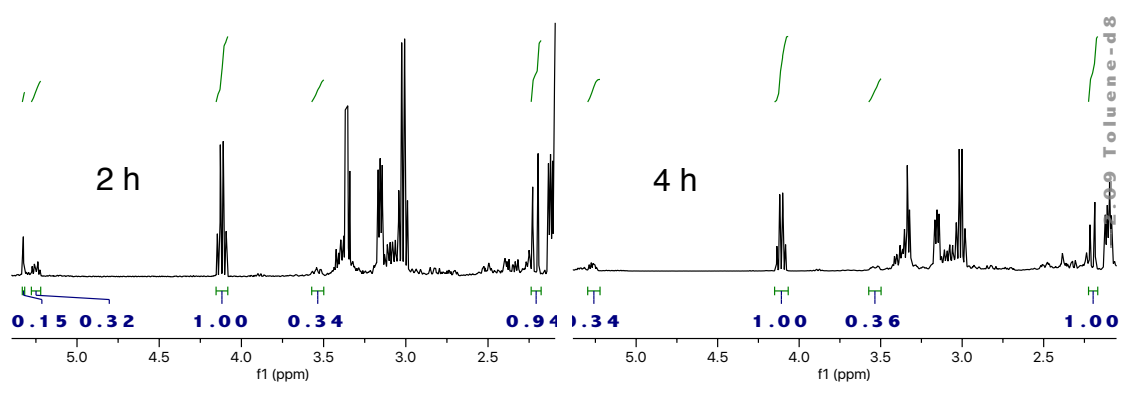
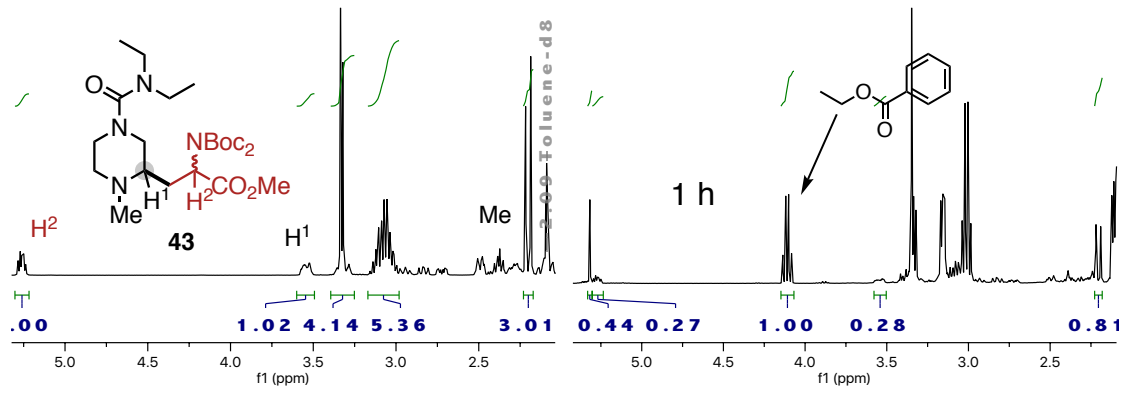
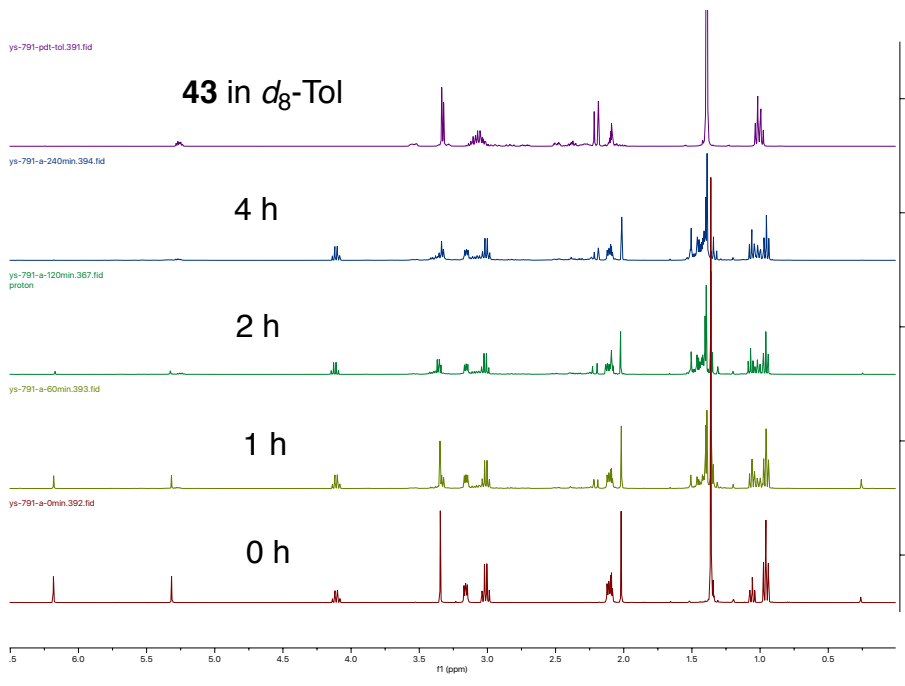
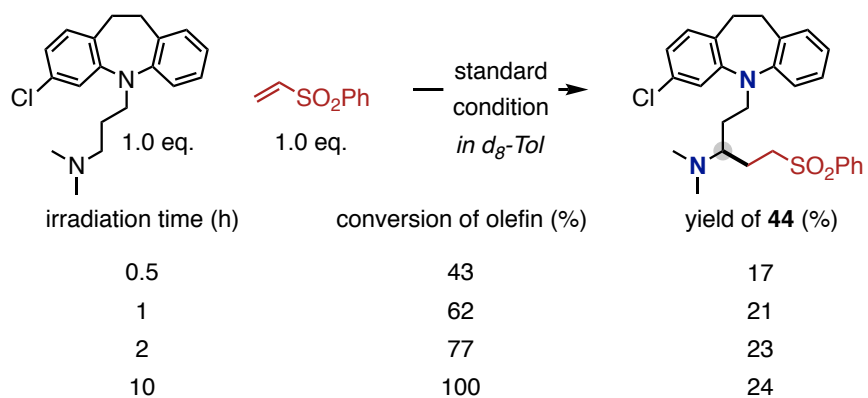
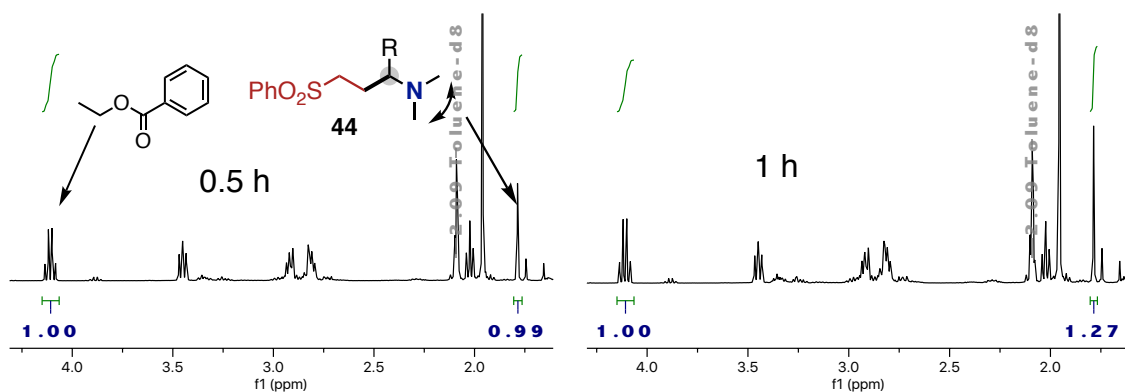
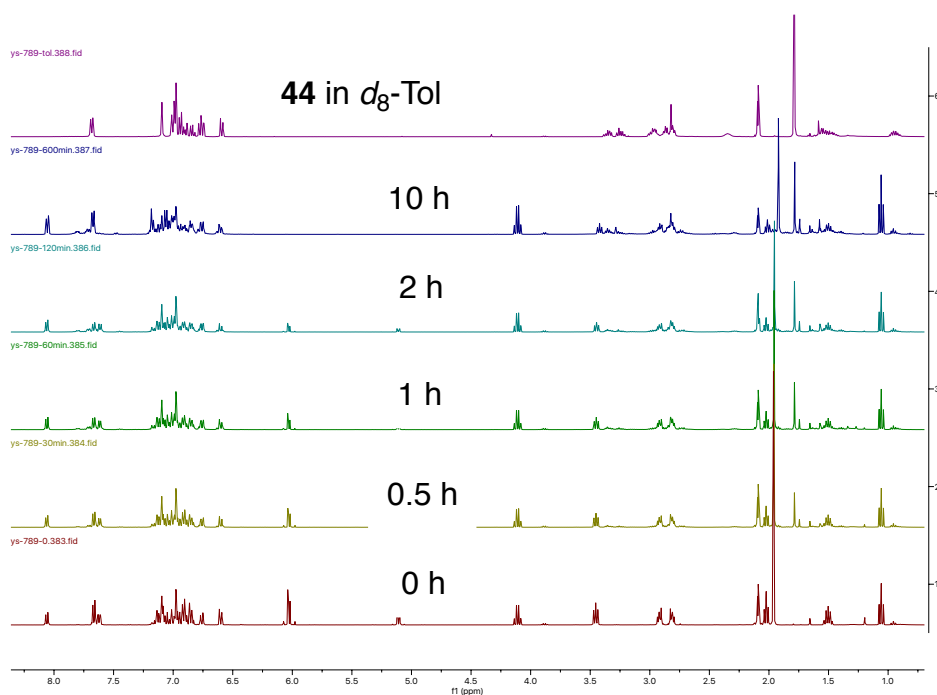
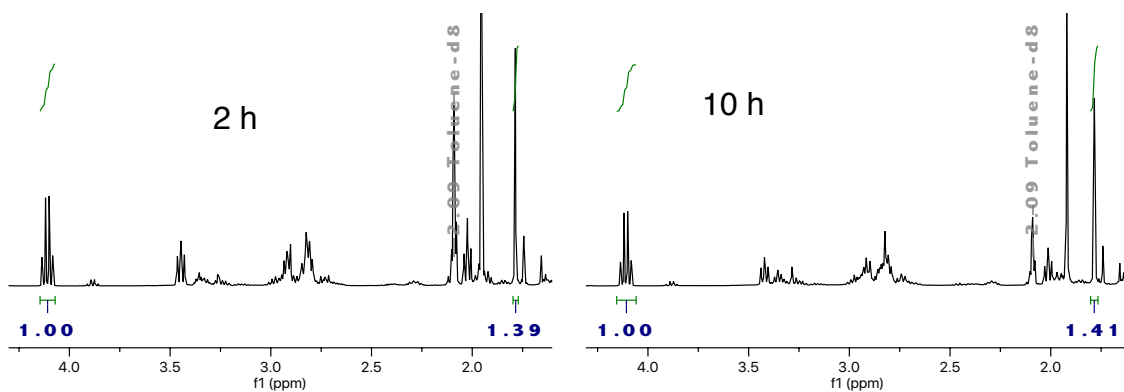


Table S7. Practical consideration of alkylation of clomipramine



0.2 mmol scale. 0.1 mmol of ethyl benzoate as internal standard.





III. Mechanistic experiments

On/Off experiments of standard reactions

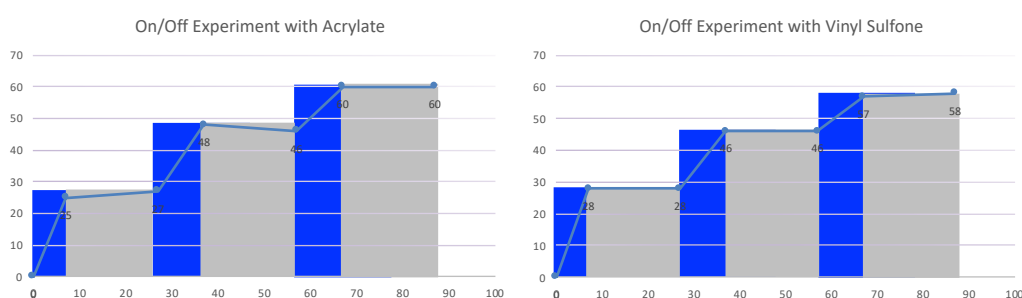


Chart 1. On/Off experiments; Y axis: Yield (%), X axis: Time (min).

Quenching Studies

Standard solution of $\text{Ir}(\text{ppy})_2(\text{dtbbpy})\text{PF}_6$ in Toluene (5.0×10^{-5} M) was used for the analysis.

Samples were irradiated at 480 nm and emission was measured at 580 nm.

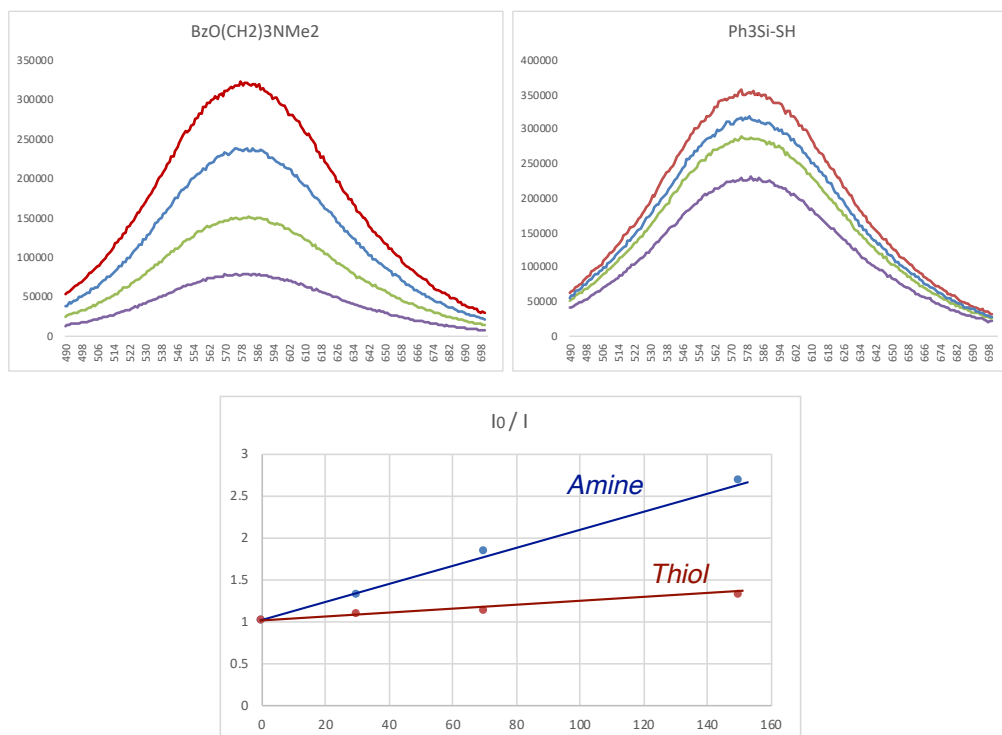


Chart 2. Quenching studies (intensity of emission at 582 nm was used).

Quantum yield calculation

Quantum yield was calculated according to reported literature.¹

The measurement of the photon flux (11 cm away from light source) at maximum intensity of a Kessil PR160 (34W maximum, 240 VDC, 440 nm) was determined by standard ferrioxalate actinometry following already reported procedures (average of 3 measurements).

Photon flux (average of 3 times) = 4.32×10^{-9} einstein·s⁻¹

A cuvette was charge with standard reaction solution and then placed 11 cm away from the light source. (Under these conditions, the fraction of light absorbed by the photocatalyst was $f = 0.965$) The sample was irradiated for 420 s (7 min). Product was detected with GC-MS in (18+20+21)/3% yield. The quantum yield was calculated as 23.

$$\Phi = \frac{\text{mol of Product}}{\text{flux} \times t \times f} = \frac{0.2 \times 0.2 \times 10^{-3} \text{ mol}}{4.32 \times 10^{-9} \text{ einstein} \cdot \text{s}^{-1} \times 420 \text{ s} \times 0.965} \approx 23$$

Control studies under thermal conditions:

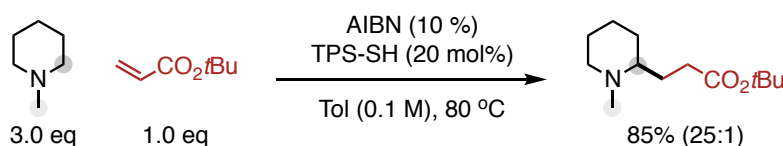
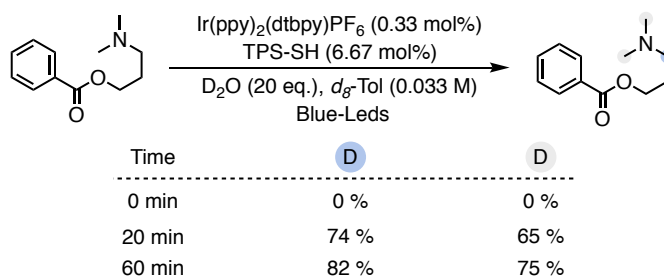


Fig. S1. Control experiment with catalytic amount of AIBN

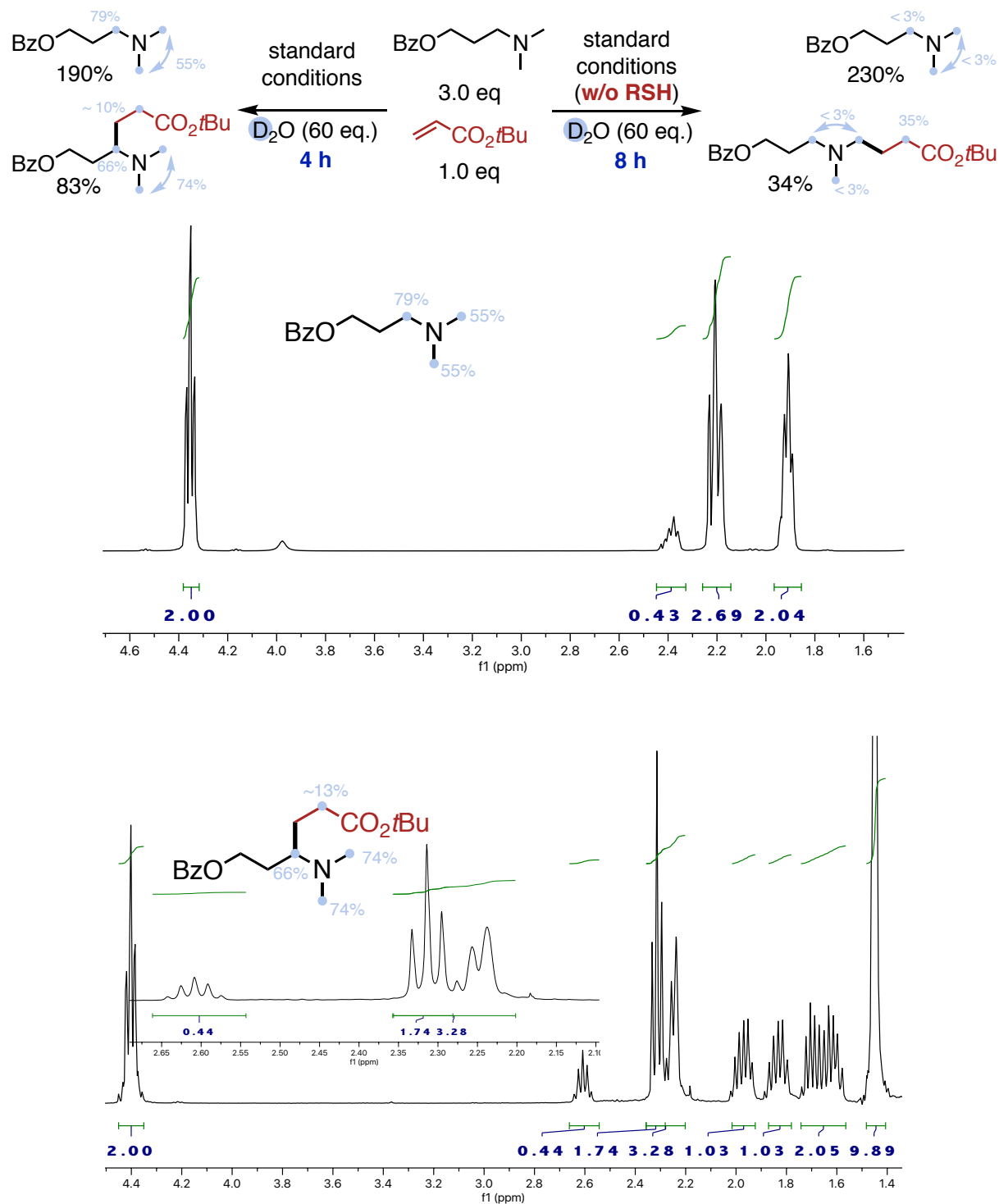
Deuteration studies under various conditions:

Table S8. Deuteration studies with different period of irradiation time



D₂O (60 eq., 220 μL, 12 mmol) was added to the reaction mixture. After 10 min, the reaction was removed from the light source and TLC showed *the alkene was not fully consumed*. Then the mixture was directly purified by flash column chromatography in silica gel with CHCl₃/MeOH and the results were analyzed by NMR.

D₂O (60 eq., 220 μL, 12 mmol) was added to the standard reaction. As a control, D₂O (60 eq., 220 μL, 12 mmol) was added to the standard reaction without TPS-SH. After indicated time, the mixture was directly purified by flash column chromatography in silica gel with CHCl₃/MeOH and the results were analyzed by NMR and shown below.



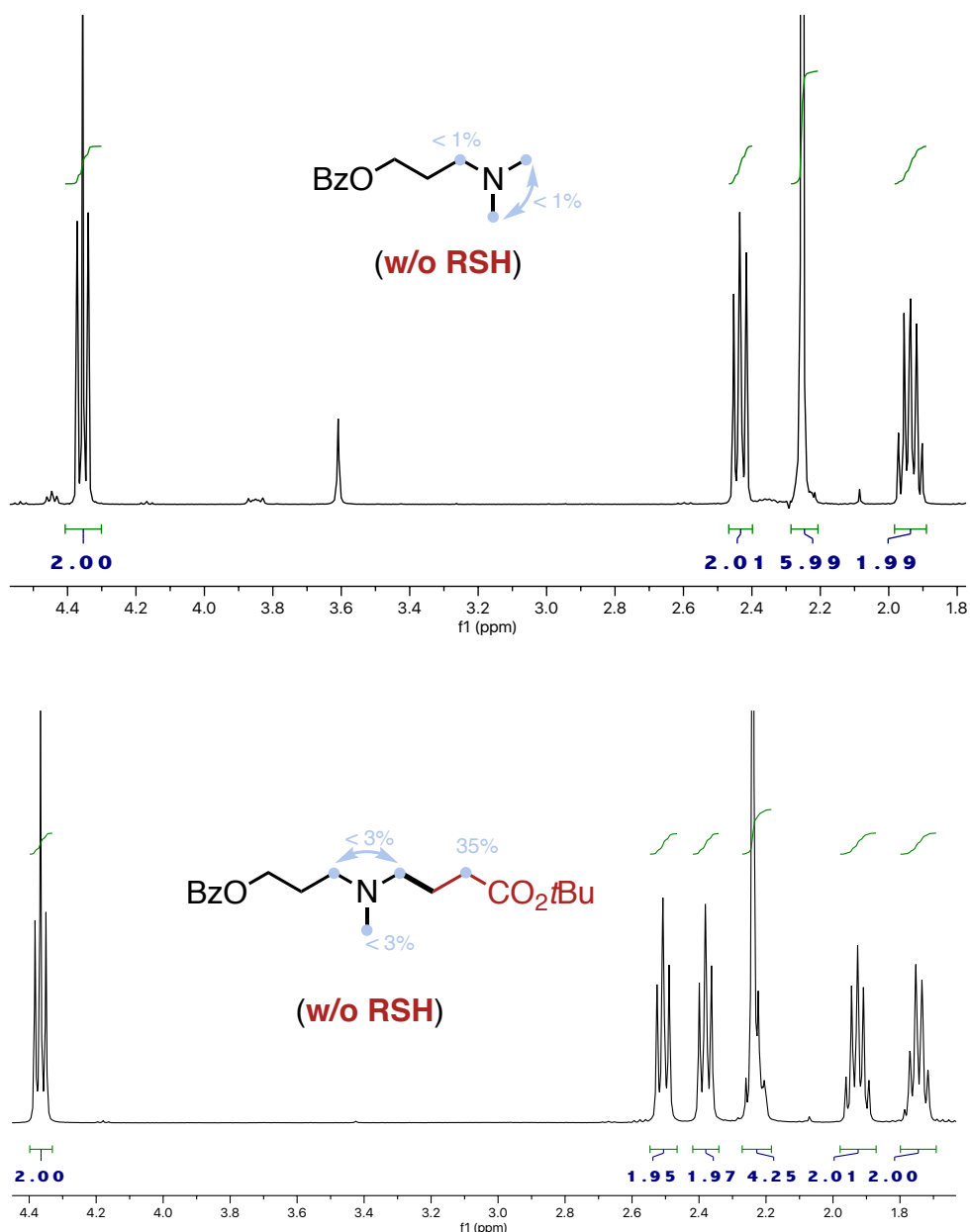


Fig. S3. Deuteration studies with acrylate with or w/o RSH under irradiation

AIBN (10 mol%, 3.3 mg, 0.02 mmol), TIPS-SH (20 mol%, 8.6 μ L, 0.04 mmol) and D₂O (60 eq., 220 μ L, 12 mmol) in *m*-Xylene (0.1 M) were used, the reaction was stirred in preheated oil-bath (80 °C). After 4 h, the mixture was directly purified by flash column chromatography in silica gel with CHCl₃/MeOH and the results were analyzed by NMR.

(Note: We found in toluene at 80 °C, the added D₂O evaporates quickly and condenses on the sides of the reaction vessel. The same issue remains in m-xylene, but with some D₂O evident at the bottom.)

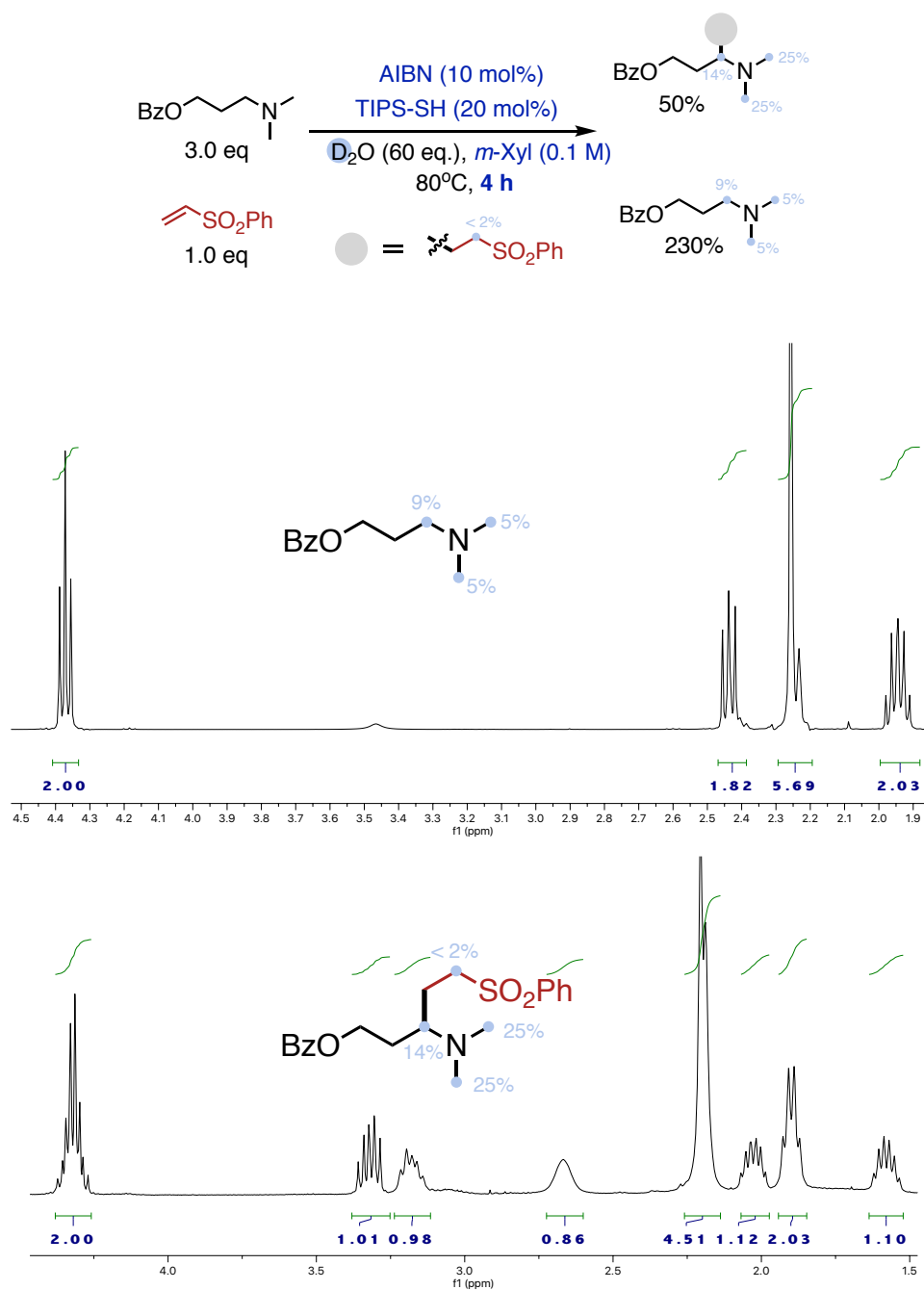


Fig. S4. Deuteration studies with vinyl sulfone under heating

AIBN (10 mol%, 3.3 mg, 0.02 mmol), TIPS-SH (20 mol%, 8.6 μL , 0.04 mmol) and D_2O (60 eq., 220 μL , 12 mmol) in *m*-Xylene (0.1 M) were used, the reaction was stirred in preheated oil-bath (80 °C). After 4 h, the mixture was directly purified by flash column chromatography in silica gel with $\text{CHCl}_3/\text{MeOH}$ and the results were analyzed by NMR.

(Note: We found in toluene at 80 °C, the added D_2O evaporates quickly and condenses on the sides of the reaction vessel. The same issue remains in *m*-xylene, but with some D_2O evident at the bottom.)

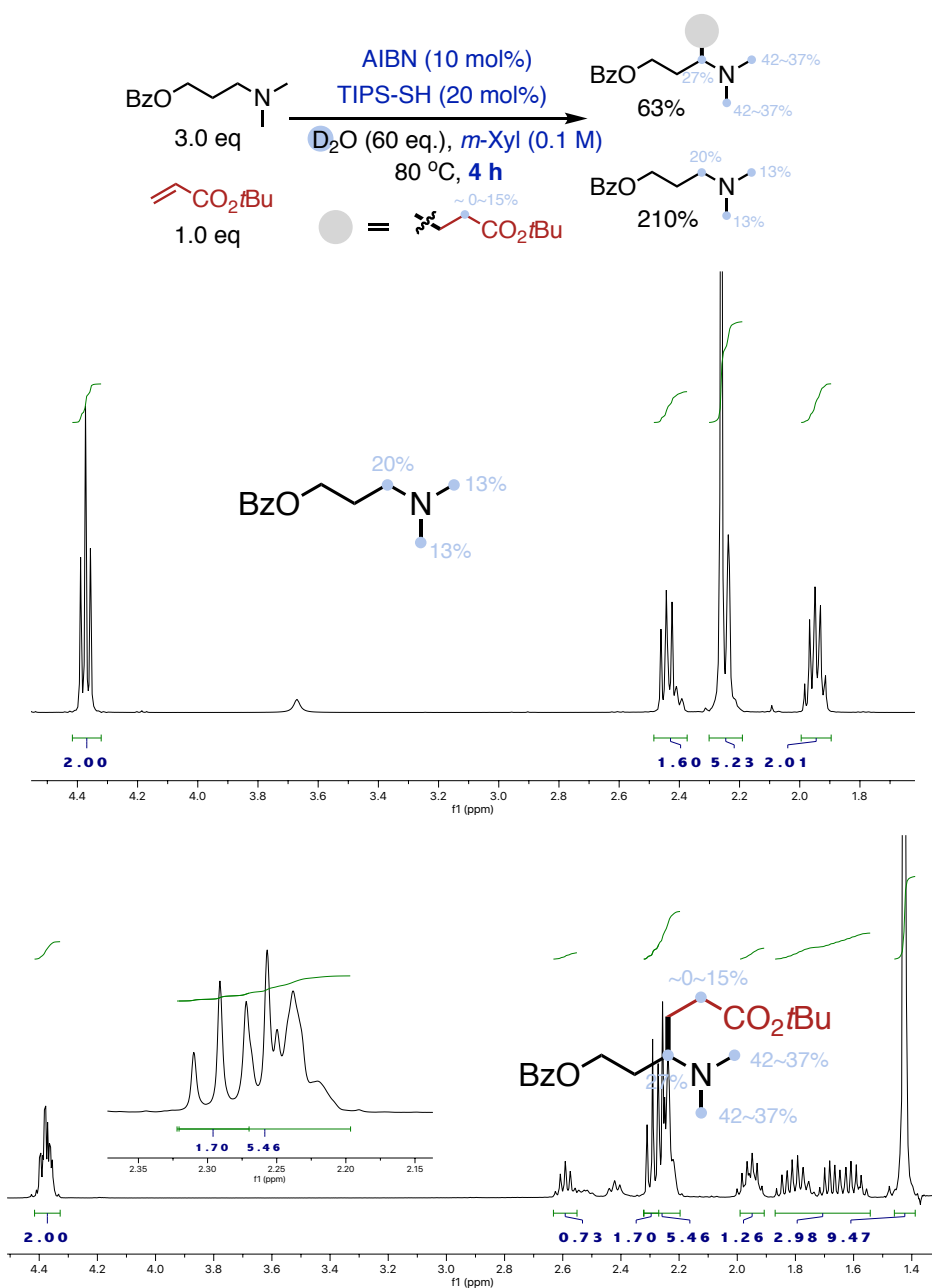


Fig. S5. Deuteration studies with acrylate under heating

Cyclic Voltammetry Studies

Cyclic voltammetry (CV) studies were performed on a CH instruments Model 1232B potentiostat. All experiments were run using an EDAQ 1-mm disk glassy carbon working electrode in conjunction with an EDAQ Ag/AgCl reference electrode. Platinum wire from VWR served as the counter electrode. All voltammetry measurements were run in anhydrous acetonitrile from Sigma-Aldrich at 50 mM (5 mM for photocatalyst) using tetrabutylammonium hexafluorophosphate (0.1 M) as the electrolyte under a gentle flow of N_2 . The scan rate was set

at 100 mV/s with a sensitivity of 1.0×10^{-4} . X-axis as Potential (V), Y-axis as Current (A). CV data of $i\text{Pr}_3\text{SiSH}$ is known ($E_{1/2}^{\text{ox}} = 0.28 \text{ V vs Ag/AgCl}$ in MeCN).²

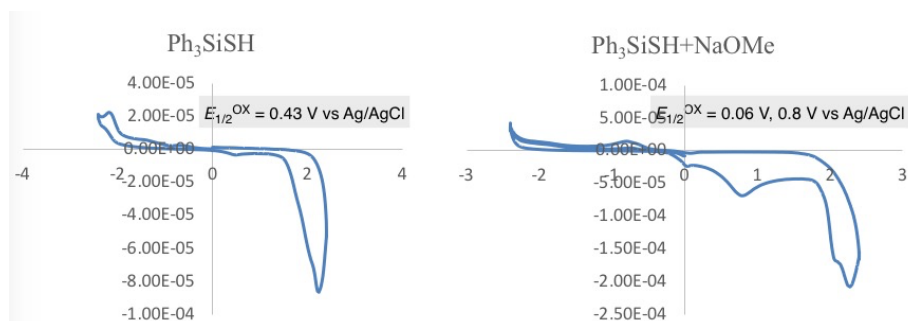


Fig. S6. CV of Ph_3SiSH with or w/o NaOMe

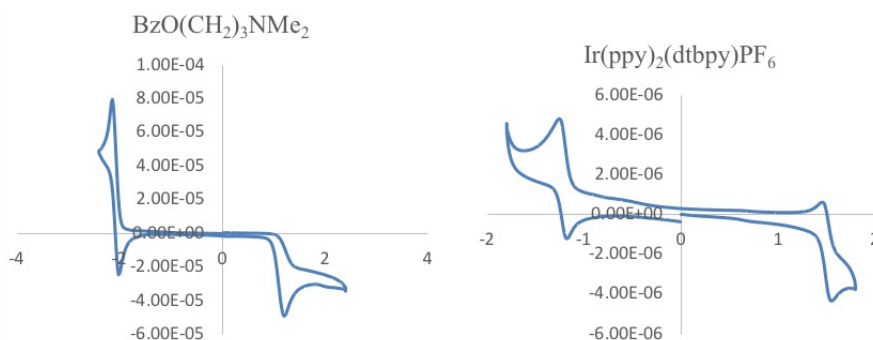


Fig. S7. CV of $\text{BzO}(\text{CH}_2)_3\text{NMe}_2$

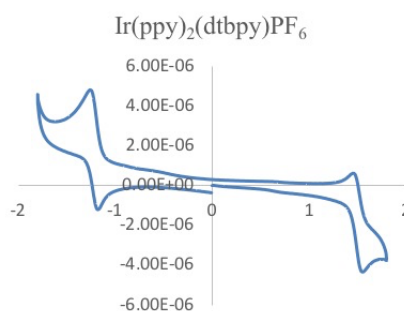


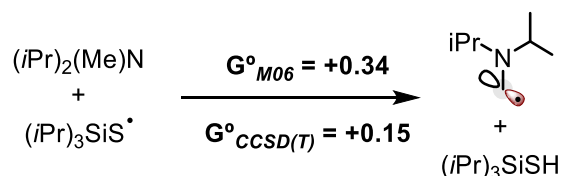
Fig. S8. CV of $\text{Ir}(\text{ppy})_2(\text{dtbbpy})\text{PF}_6$

IV. Computational details

DFT calculations were carried out with using Gaussian16 program package (v A.03).³ All structures were optimized using the M06 functional and 6-31+G(d,p) basis set, which is convenient for organic molecules with open-shell electronic structure, including implicit solvation (toluene) by CPCM method. Frequency calculations were conducted at the same level of theory to corroborate the nature of stationary points as minima (zero imaginary frequencies) or transition state (one imaginary frequency). Transition states were also confirmed by IRC calculations and relaxation towards reactants and products. The potential energy was further refined using the same method together with the 6-311++G(3d,2p) basis set. Finally, 1M standard state (addition of 1.89 kcal/mol) correction was added to all species.

3D images were created by CYLview software.⁴

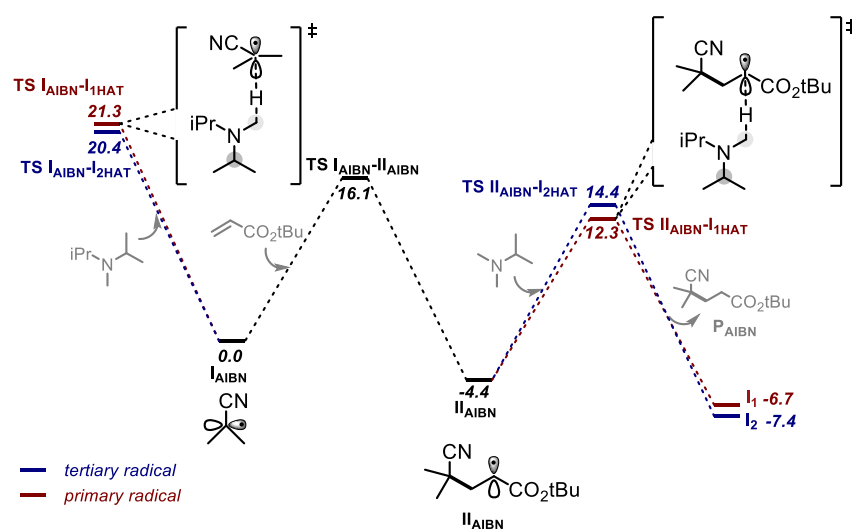
Radical stability of primary radical of $(i\text{Pr})_2(\text{Me})\text{N}$ vs $(i\text{Pr})_3\text{Si-SH}$ radical was benchmarked, comparing the DFT results with CCSD(T) (+ DFT G_{Corr} + DFT G_{Solv}). Both methodologies yield similar results, confirming the reversibility of the process.



For Fig. 4 in the main text, all the calculations were carried out at the same level of theory. The starting geometries of pharmaceuticals were taken from CCDC (Cambridge Crystallographic Data Centre) for all compounds except Clormipramine (not available). ^{13}C NMR shifts were calculated using the GIAO method and they are referenced to TMS (calculated at the same theory level).

Free energy profiles of complete reaction pathway with and without HAT catalyst:

Initiation without $(\text{iPr})_3\text{SiSH}$



Initiation with $(\text{iPr})_3\text{SiSH}$

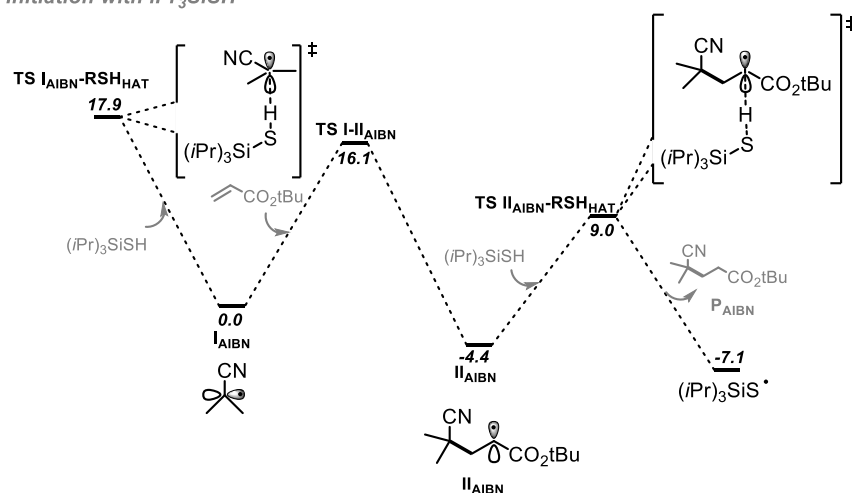


Fig. S9. Free energy (kcal/mol) profile of the initiation mechanism under HAT-catalyst free conditions (top) and with $(\text{iPr})_3\text{SiSH}$ as HAT catalyst (bottom).

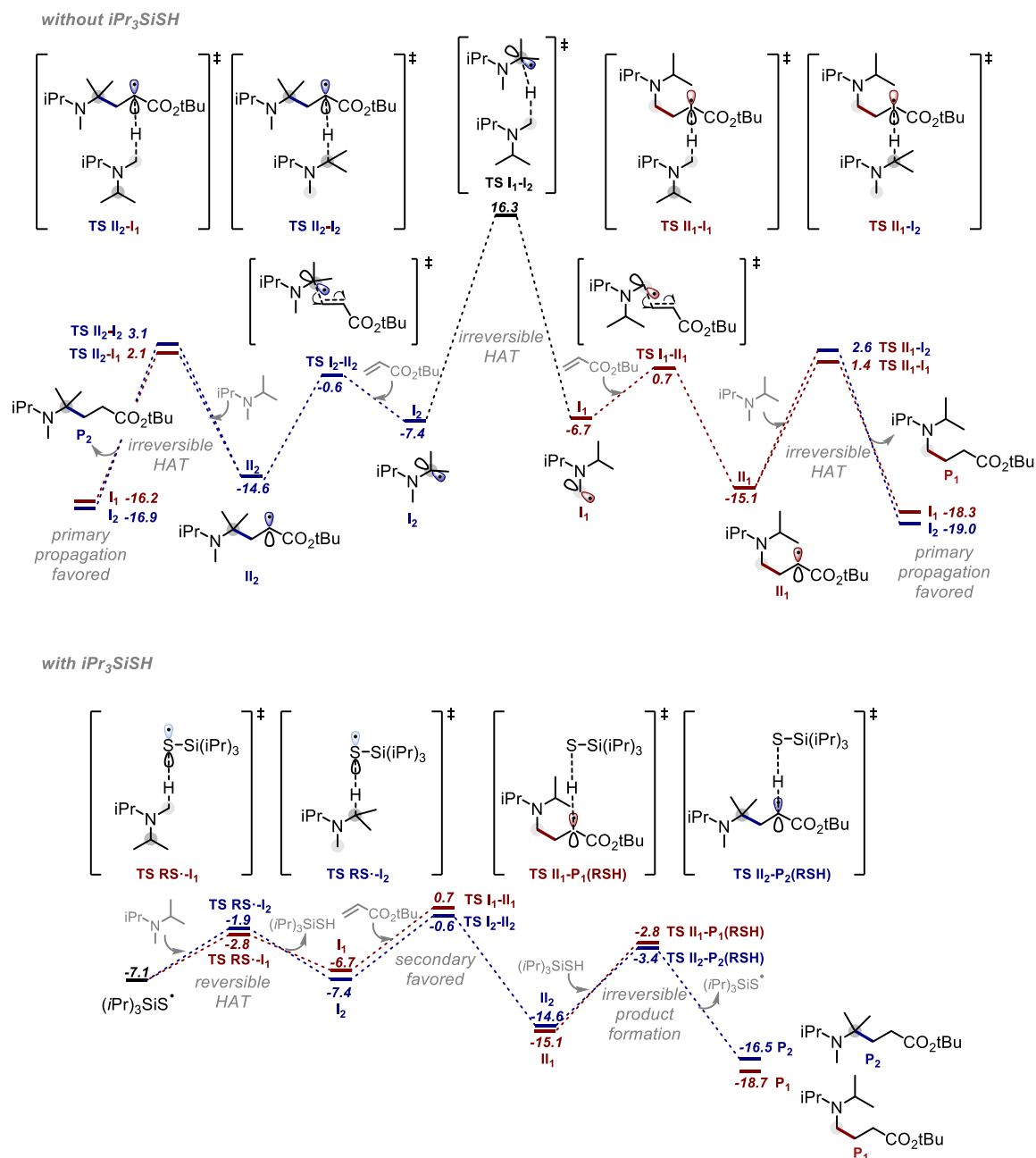


Fig. S10. Free energy profile of radical propagation without HAT catalyst and with $(i\text{Pr})_3\text{SiSH}$ as HAT catalyst (bottom). Free energies in kcal/mol.

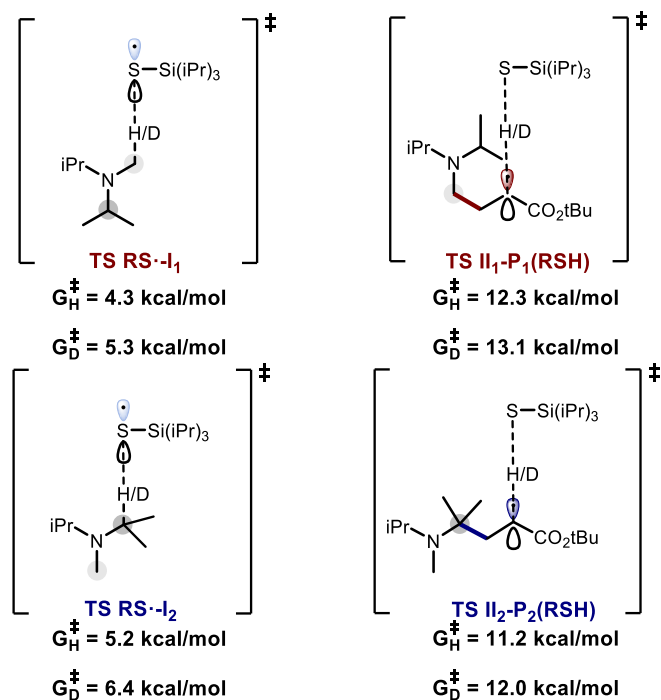


Fig. S11. Deuterium effect in HAT free energy barriers. Free energies in kcal/mol.

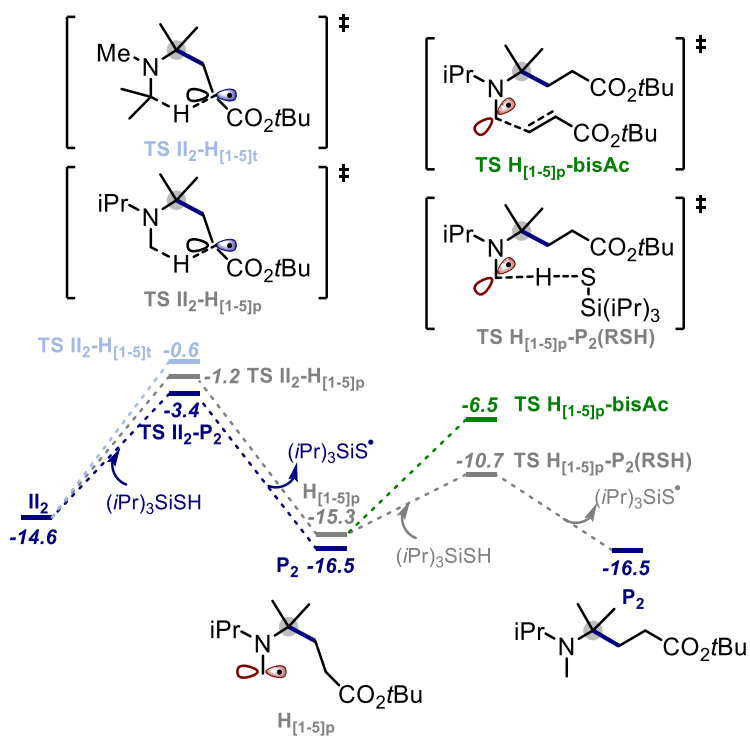


Fig. S12. Intramolecular [1,5] H-shift vs direct reaction with HAT catalyst. Free energies in kcal/mol.

	$(iPr)_3SiSH$ HAT	α -ester HAT
Tertiary		
G_{Add}^\ddagger	5.1	17.2
E_{Add}^\ddagger	-0.5	8.3
E_{Dist}	35.7	19.8
E_{int}	-35.2	-11.6
Primary		
G_{Add}^\ddagger	4.3	16.5
E_{Add}^\ddagger	-2.1	7.3
E_{Dist}	39.0	18.7
E_{int}	-41.1	-11.4

Fig. S13. Distortion interaction analysis of HAT reaction of $(iPr)_2(Me)N$ and silanethiyl radical or α -ester radical II on primary and tertiary positions. Energies in kcal/mol.

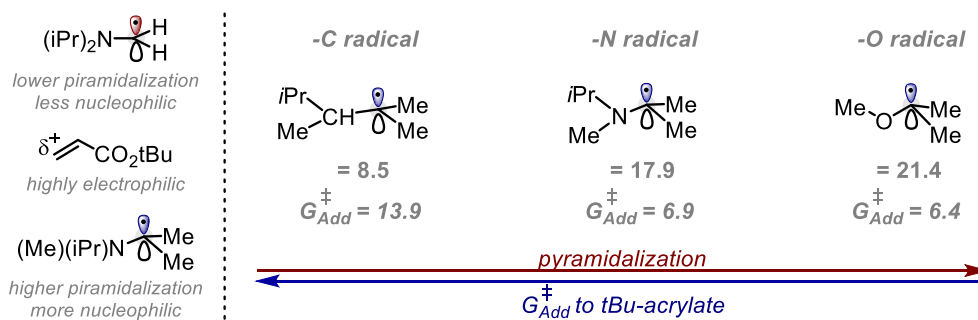


Fig. S14. Correlation between pyramidalization of radical and free energy barrier in radical addition to *t*Bu-acrylate. Free energies in kcal/mol.

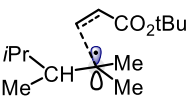
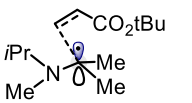
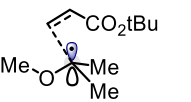
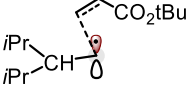
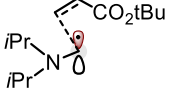
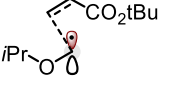
	-C radical	-N radical	-O radical
Tertiary			
G_{Add}^\ddagger	13.9	6.9	6.4
E_{Add}^\ddagger	0.8	-5.5	-5.4
E_{Dist}	7.9	5.3	2.8
E_{Int}	-7.2	-11.9	-8.2
Primary			
G_{Add}^\ddagger	10.6	7.5	8.1
E_{Add}^\ddagger	-2.4	-3.8	-3.4
E_{Dist}	3.6	1.8	2.8
E_{Int}	-6.0	-5.6	-6.2

Fig. S15. Distortion interaction analysis of radical addition to *t*Bu-acrylate of α -C, α -N and α -O primary and tertiary radicals. Energies in kcal/mol.

Distortion-interaction analysis of the different radical addition transition states show that α -O and α -N tertiary transition states have a significantly smaller distortion energy. In addition, their pyramidalization favours the interaction of the radical fragment with the double bond, resulting in a lower activation energy barrier.

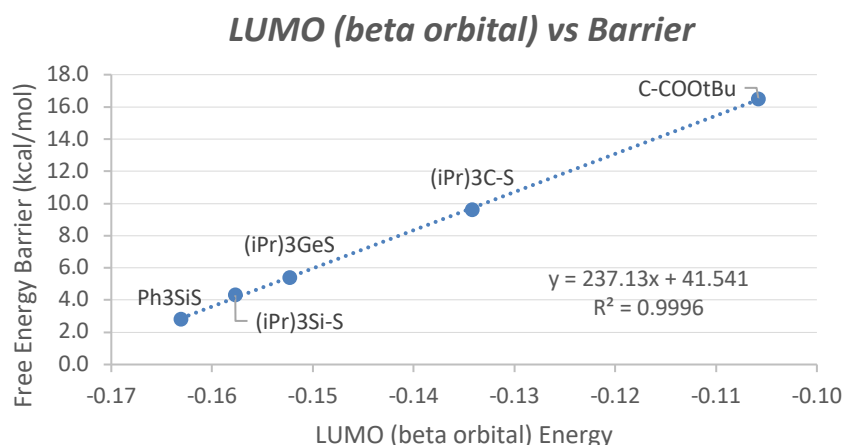


Fig. S16. Correlation between LUMO orbital of the radical and the free energy barrier of HAT from the primary site of $(iPr)_2(Me)N$ to the corresponding radical.

In order to show that the HAT catalyst reacts as an electrophilic radical, we calculated the LUMO energy of the HAT catalyst radical and its correlation with the free energy barrier for

the HAT at the primary position of substrate **3**. Interestingly, there is a linear correlation of both parameters; the electrophilicity lowers the barrier considerably. The two best catalysts (Ph_3SiSH and $(i\text{Pr})_3\text{SiSH}$) promote the HAT with a very low free energy barrier due to the polarity match in the transition states. In contrast, nucleophilic radicals, such as the α -ester radical ($\text{C-COO}t\text{Bu}$), show a significant increase of the activation barrier for HAT.

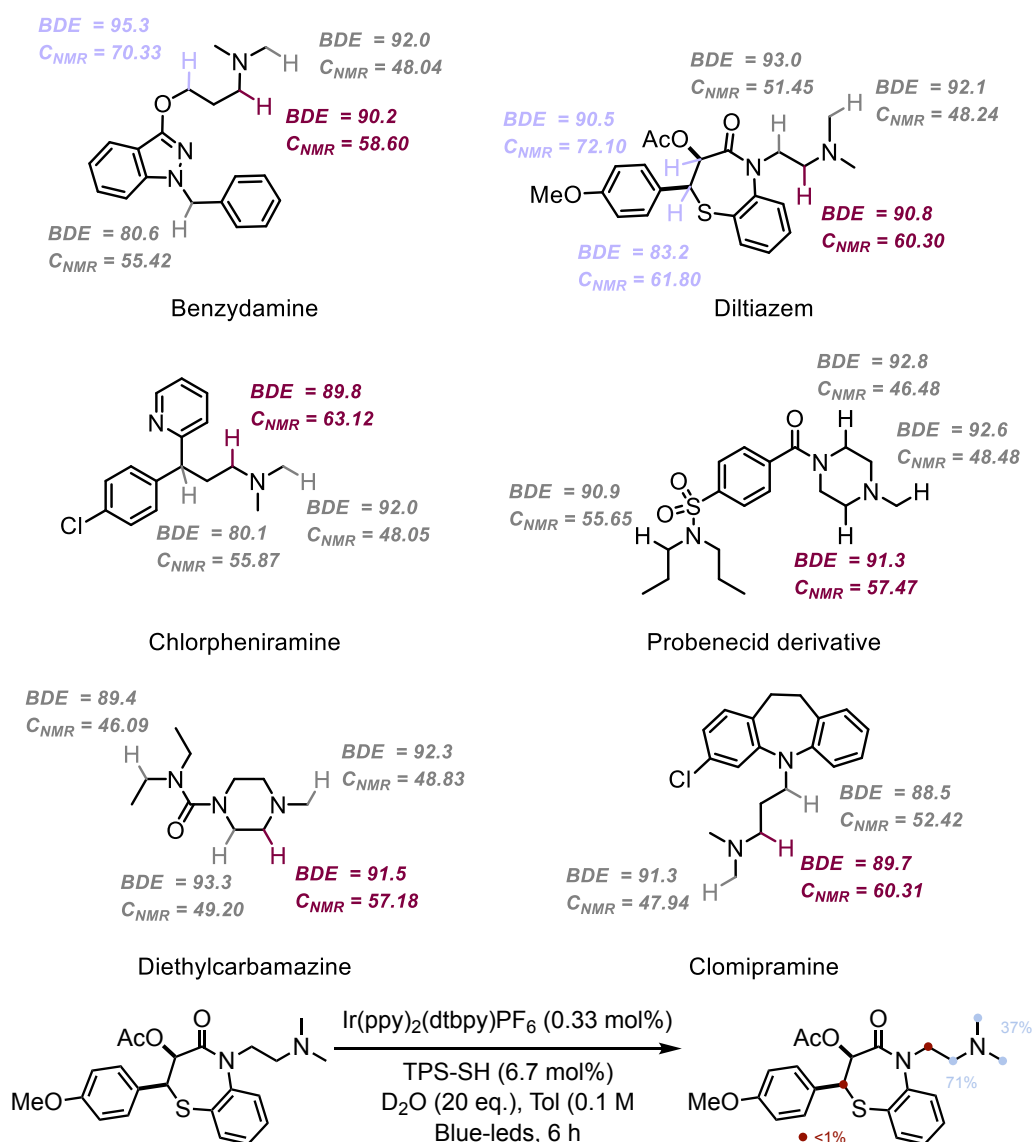


Fig. S17. Correlation between calculated C_{NMR} shifts and site selectivity in late-stage drug functionalization.

Correlation is only observed for α -N carbon centres. In the case of other heteroatoms (O, S), this correlation does not occur due to a non-reversible C-H activation mechanism, as shown in the deuteration experiment.

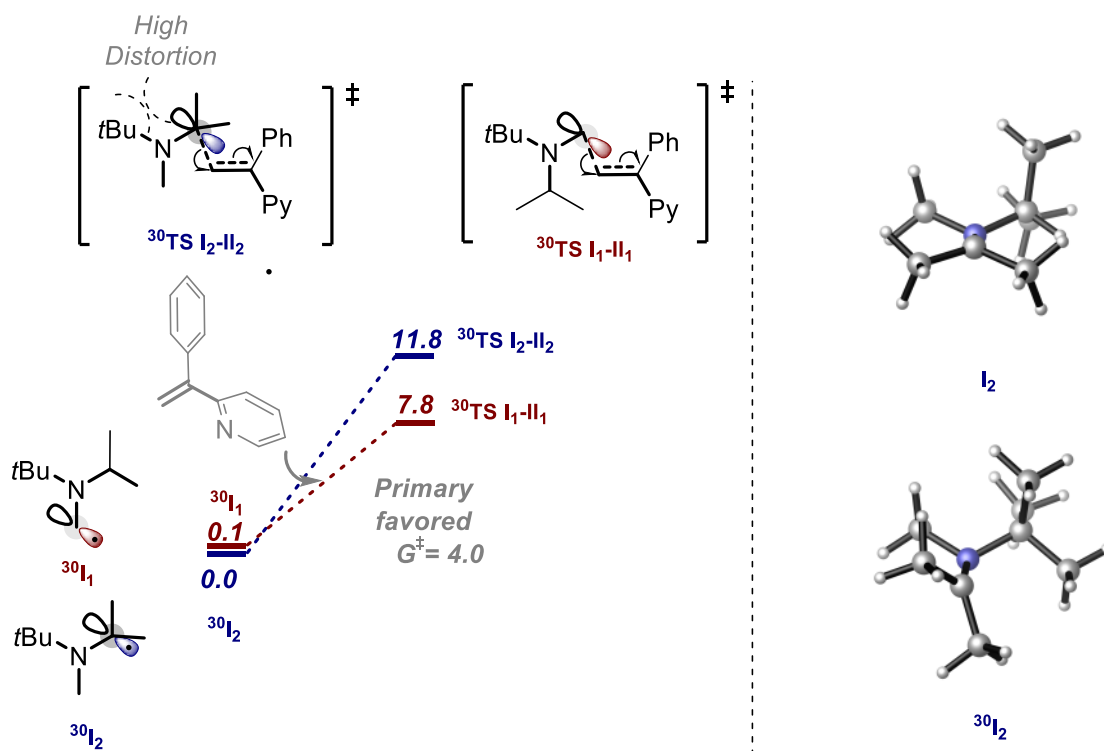


Fig. S18. Inversion of the selectivity for radical addition to product 30 in reaction with 1-phenyl-1-pyridineethane (left). Free energies in kcal/mol. 3D structures of the corresponding tertiary radical (right).

Interestingly, products **30** and **31** exhibit an opposite selectivity with respect to all the other substrates. In those cases, the least hindered position (methyl) reacts faster than the corresponding tertiary position (isopropyl). Intrigued by these exceptions, we calculated the radical addition to the alkene. We reproduced the observed selectivity inversion. The inversion is due to the *t*Bu substituent which distorts the tertiary radical structure considerably (and hence raises its energy).

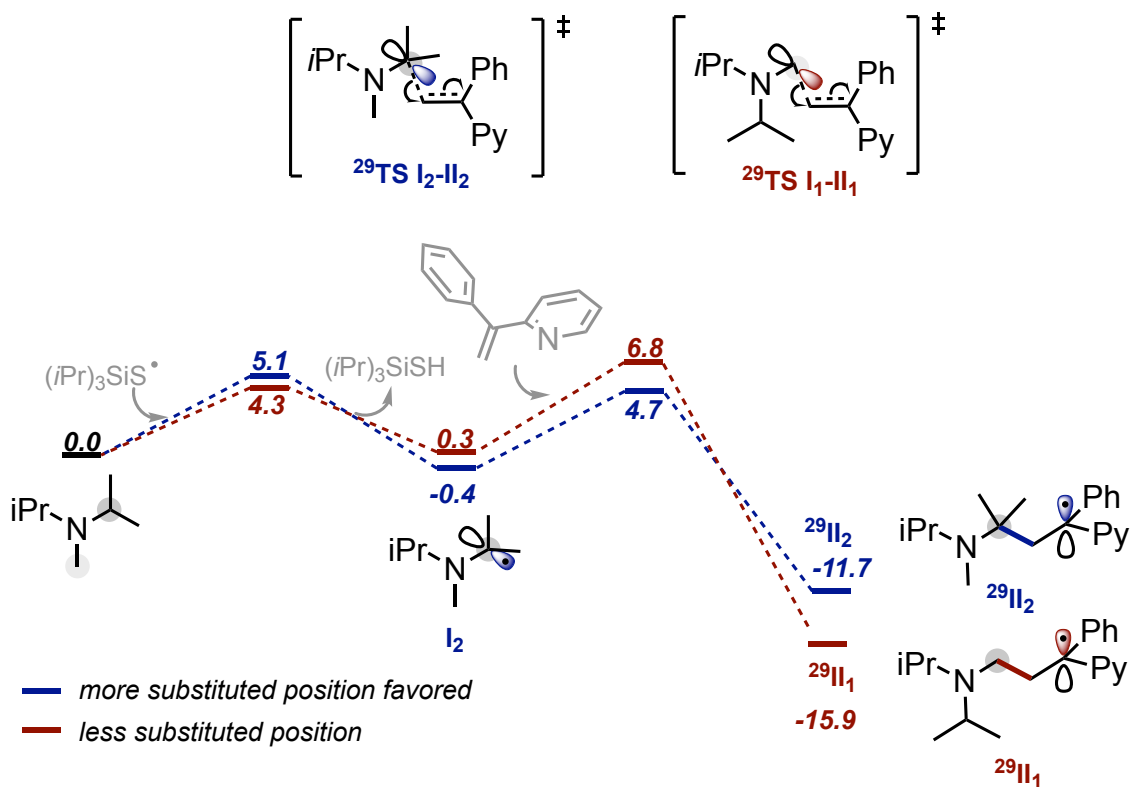
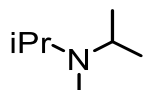


Fig. S19. Low the selectivity for radical addition to product 27 in reaction with 1-phenyl-1-pyridineethane.

In the case of the reaction with less substituted tertiary amines and diarylethylenes as radical acceptor, the radical addition barrier is decreased and starts to compete with the radical generation via reversible HAT process. Thus, the selectivity of those system is reduced (<3:1) as the reversibility of HAT is less pronounced.

XYZ Coordinates of calculated species including potential energy in solvent at high basis set and free energy correction (and enthalpy correction for BDE calculation when needed):

N(Me)(iPr)₂



E = -331.5660948

G_{Corr.} = 0.196476

H_{Corr.} = 0.242820

N	0.01044200	-0.49602600	0.01558100
C	0.03259500	-0.77059500	1.43709000
H	-0.91443600	-1.23353100	1.73789000
H	0.82278500	-1.49065500	1.67609900
H	0.18155100	0.11968000	2.07789700
C	1.25082400	0.05059100	-0.54437000
C	2.43137200	-0.86942000	-0.26493600
C	1.59010800	1.48231900	-0.12206100
H	1.09520500	0.05347500	-1.63566500
H	2.17794000	-1.91250000	-0.48687900
H	3.28570200	-0.57982100	-0.88740900
H	2.75904300	-0.80733900	0.78108000
H	0.82979600	2.19883200	-0.45307300
H	1.68753200	1.56344400	0.96908800
H	2.54736100	1.79038300	-0.56111000
C	-1.22570200	0.13507500	-0.46671500
C	-1.78566100	1.25342900	0.41576700
C	-2.29717800	-0.92245200	-0.70705900
H	-0.97096000	0.57563200	-1.44375400
H	-1.03407800	2.01180600	0.66090900
H	-2.61563600	1.75388300	-0.09758100
H	-2.18181900	0.85526300	1.35916200
H	-1.94029400	-1.68396000	-1.40854400
H	-2.57037000	-1.42610300	0.22999700
H	-3.21056200	-0.46998300	-1.11346400

tBu-Acrylate



E = -424.2704695

G_{Corr.} = 0.142635

C	-3.48113800	0.20164900	-0.00007500
C	-2.26501700	0.74558800	0.00003600
H	-4.37852400	0.81320400	-0.00007700
H	-3.60048600	-0.87993800	-0.00016200
H	-2.10963900	1.82205300	0.00013300
C	-1.05278100	-0.10747400	0.00006600
O	-1.06480000	-1.32304000	0.00001900
O	0.04640600	0.65565600	0.00010200
C	1.39544900	0.07385800	-0.00001700
C	1.60916800	-0.74134900	1.26377700
C	1.60932400	-0.74066200	-1.26423200
C	2.28839600	1.30140600	0.00035700
H	1.38072800	-0.13702200	2.14974300
H	0.98975700	-1.64162600	1.27655900
H	2.66233000	-1.04174000	1.32062900
H	1.38091800	-0.13587500	-2.14989300
H	2.66251500	-1.04094200	-1.32115600
H	0.98998900	-1.64097800	-1.27755700

H	3.34080900	0.99588000	0.00033000
H	2.10421500	1.91422000	-0.88935100
H	2.10412400	1.91374700	0.89037200

I_{AIBN}

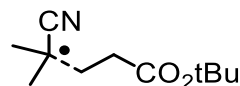


E = -210.6417195

G_{Corr.} = 0.056627

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H	0.00086800	-0.40230800	2.15758200
H	-0.88071400	-1.71750200	1.34654300
H	0.88051100	-1.71813400	1.34544700
C	-0.00037100	-0.31118000	0.00000000
C	0.00008000	-1.06242900	-1.28687500
H	0.00086800	-0.40230800	-2.15758200
H	0.88051100	-1.71813400	-1.34544700
H	-0.88071400	-1.71750200	-1.34654300
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N	0.00008000	2.25740200	0.00000000

TS I_{AIBN}-II_{AIBN}



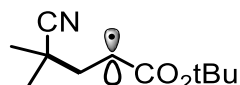
E = -634.9068043

G_{Corr.} = 0.222495

C	-2.79747600	0.50846100	0.20573800
C	-1.64048100	-0.85845800	-1.09841800
H	-1.72476400	-1.68516600	-0.39380100
H	-2.40212400	-0.79133100	-1.87209600
C	-0.41700500	-0.27765700	-1.29070900
H	-0.24628600	0.45071500	-2.08091500
C	0.69893000	-0.56003200	-0.37854800
O	0.65532400	-1.36630300	0.53509500
O	1.76203500	0.19732100	-0.68987500
C	3.00220700	0.14704900	0.09289600
C	2.72653000	0.58665300	1.52117200
C	3.61663500	-1.24024300	0.01550600
C	3.88588400	1.15910500	-0.61386200
H	2.23190600	1.56580600	1.52781500
H	2.10074000	-0.13361800	2.05463400
H	3.67850300	0.68473300	2.05660900
H	3.73332700	-1.54626700	-1.03091000
H	4.61244900	-1.21542400	0.47424900
H	3.01091800	-1.98387700	0.53882800
H	4.85866900	1.21804700	-0.11277500
H	4.04967600	0.86715000	-1.65738100
H	3.42544400	2.15352000	-0.59756100
C	-1.94925800	0.62474300	1.43533400
H	-1.76425800	-0.34544000	1.90620800
H	-0.98475100	1.08275800	1.18446500
H	-2.44356000	1.27648200	2.17037600
C	-2.94280000	1.73284500	-0.64786200
H	-3.50632800	2.50516800	-0.10466000
H	-1.95500900	2.14624200	-0.88102000

H	-3.47303900	1.52610600	-1.58305700
C	-3.94027600	-0.33002800	0.30075400
N	-4.85681900	-1.05405300	0.34103100

II_{AIBN}

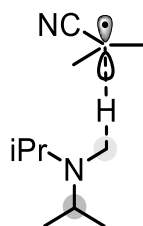


$$E = -634.9429005$$

$$G_{\text{Corr.}} = 0.226071$$

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H	-1.63403600	-1.30943700	-0.86988000
H	-2.23387500	-0.02614500	-1.94695700
C	-0.44246400	0.43626400	-0.90967900
H	-0.30825000	1.45905800	-1.25746700
C	0.72165400	-0.25936100	-0.38132300
O	0.69405800	-1.40550300	0.04343600
O	1.80879100	0.52807500	-0.42013200
C	3.11144000	0.07034600	0.07789200
C	3.01988200	-0.23612700	1.56326000
C	3.59150100	-1.11980000	-0.73534200
C	4.00365200	1.27455200	-0.16291500
H	2.60471900	0.62292200	2.10407200
H	2.40104300	-1.11513200	1.76004200
H	4.02762100	-0.42626600	1.95166600
H	3.58376600	-0.87781700	-1.80476300
H	4.62344500	-1.35509000	-0.44841300
H	2.97333600	-2.00484500	-0.56501300
H	5.02346500	1.05485500	0.17248500
H	4.03504600	1.52578800	-1.22915700
H	3.63585900	2.14590200	0.39075900
C	-2.18731900	-0.05168300	1.52867100
H	-1.95643500	-1.11694500	1.63383400
H	-1.26290300	0.51722800	1.68928000
H	-2.90376900	0.23383900	2.30636600
C	-3.03536400	1.76147100	0.00092500
H	-3.78513400	2.07769500	0.73406000
H	-2.11932700	2.33410700	0.18620700
H	-3.40559800	2.00729700	-1.00086500
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N	-4.99623800	-1.05397000	-0.19782800

TS I_{AIBN}-I_{1HAT}



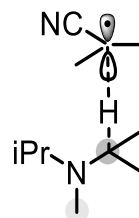
$$E = -542.189744$$

$$G_{\text{Corr.}} = 0.272013$$

N	-1.26017900	0.02814600	-0.55865400
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H	-0.02749900	-0.32738100	-2.19976800
H	-0.09710700	1.39495500	-1.62929700
H	1.03756200	0.15947500	-0.69405800
C	-1.78445200	1.04469400	0.36186100
C	-2.60685500	2.07664800	-0.40018700
C	-0.70070100	1.70450500	1.20807700
H	-2.46303700	0.51556000	1.04458400
H	-3.41612300	1.59318600	-0.95941600
H	-3.04626500	2.80618300	0.29029800

H	-1.98242200	2.62992500	-1.11369500
H	-0.11806100	0.96777100	1.77263200
H	-0.00450300	2.28276600	0.58549800
H	-1.15662800	2.40142100	1.92092600
C	-1.51383200	-1.38647000	-0.27132800
C	-2.99924500	-1.70972000	-0.35648200
C	-0.91324400	-1.83921300	1.05596600
H	-1.00418000	-1.93559200	-1.07797700
H	-3.41293200	-1.39960400	-1.32247800
H	-3.15768900	-2.78804400	-0.24002300
H	-3.56989200	-1.21059100	0.43721000
H	0.15951100	-1.61821200	1.11077800
H	-1.40199100	-1.34351600	1.90503400
H	-1.04756800	-2.91987100	1.18437500
C	3.02699600	1.20220900	-0.94251500
H	2.70925000	2.11973400	-0.43404800
H	4.12384600	1.14874800	-0.89464700
H	2.74541400	1.28303500	-2.00118700
C	2.37780200	-0.02511700	-0.34096300
C	2.71285100	-1.32904000	-1.03298700
H	2.15230100	-2.17080500	-0.60900000
H	2.46155000	-1.25434700	-2.09921800
H	3.78409200	-1.56444500	-0.96116300
C	2.40136900	-0.08446700	1.08107500
N	2.34980300	-0.13334400	2.25015900

TS I_{AIBN}-I_{2HAT}



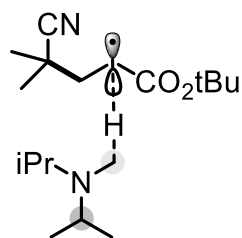
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$$G_{\text{Corr.}} = 0.271773$$

N	-1.34305400	0.43331300	0.43573600
C	-1.55785400	0.03015100	1.81346500
H	-2.53882700	-0.44820600	1.89915300
H	-0.79900800	-0.67917100	2.18624600
H	-1.57251600	0.90116700	2.47358300
C	-0.22667900	1.24551100	0.11544100
C	0.31339300	2.06374000	1.26443100
C	-0.40281900	2.08720700	-1.13331800
H	0.82415900	0.44867200	-0.15646200
H	0.67523600	1.44251000	2.09255500
H	1.15309000	2.67340000	0.91329900
H	-0.44995500	2.75275300	1.65774300
H	-0.76227300	1.52215500	-1.99910100
H	-1.12930600	2.89202300	-0.93853800
H	0.54826800	2.55508600	-1.41461800
C	-1.81483400	-0.52550900	-0.57990000
C	-3.28549700	-0.28926100	-0.89321500
C	-1.55085400	-1.98334900	-0.21223600
H	-1.23559300	-0.32210800	-1.48994400
H	-3.44752000	0.73409900	-1.25111700
H	-3.63841300	-0.98909400	-1.66057800
H	-3.90492800	-0.43729200	0.00127600
H	-0.51311500	-2.14609100	0.10414200
H	-2.20576500	-2.32917400	0.59674400
H	-1.74675000	-2.61934000	-1.08382300
C	3.12381400	0.68862500	-0.33515400
H	3.24813300	1.10147300	0.67185400
H	4.07875400	0.23056000	-0.63186800
H	2.93023700	1.51826900	-1.02743200
C	1.99306100	-0.31483200	-0.40060200
C	1.74930100	-0.90564200	-1.77220200
H	0.90563500	-1.60571900	-1.77479200
H	1.53109500	-0.10206000	-2.48780400
H	2.63500300	-1.44386100	-2.13970700

C	1.96191000	-1.24627300	0.67714700
N	1.85686900	-1.96935000	1.59227200

TS II_{AIBN-I₁HAT}



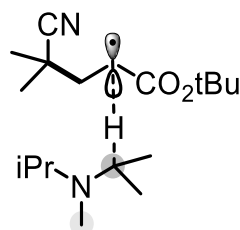
E = -966.49896

G_{Corr.} = 0.439079

C	3.37950200	-1.31347200	0.24856800
C	1.87152700	-1.50034500	-0.06890400
H	1.73976600	-1.52557000	-1.15979200
H	1.57833400	-2.49087300	0.31302500
C	0.96698700	-0.44472600	0.50291300
H	1.01938700	-0.28858700	1.58385700
C	0.80330300	0.78440200	-0.26420600
O	0.91685000	0.87179800	-1.48161300
O	0.45198700	1.81916800	0.53562100
C	0.28213400	3.17477100	0.01809500
C	1.59643700	3.67279600	-0.56193800
C	-0.85368500	3.23813600	-0.99081200
C	-0.07888700	3.96710600	1.26315900
H	2.39754100	3.57807200	0.18174000
H	1.87751900	3.11707400	-1.46069200
H	1.50013200	4.73371700	-0.82313500
H	-1.77646100	2.83476000	-0.55427500
H	-1.03839700	4.28655400	-1.25582600
H	-0.61879200	2.68171300	-1.90183500
H	-0.23094600	5.02172200	1.00598600
H	-1.00252900	3.58207900	1.71210600
O	0.72260200	3.90206600	2.00791800
N	-2.52804100	-1.52064900	0.05057300
C	-2.80952700	-1.38858200	-1.38215800
H	-2.11190600	-2.08216900	-1.87397700
C	-1.28662400	-2.00702600	0.44001400
H	-0.28944100	-1.10652000	0.41497400
C	-3.31341000	-0.73419600	1.00924800
C	-2.48655700	0.34090700	1.70525000
C	-4.00505800	-1.64743500	2.01398000
H	-4.09184800	-0.22769600	0.42309000
H	-1.95785400	0.97679400	0.98546100
H	-3.13727800	0.97629200	2.31753000
H	-1.73372800	-0.09994500	2.37210500
H	-4.64537200	-2.37606700	1.50415600
H	-3.27012400	-2.19992800	2.61360900
H	-4.62377200	-1.06223500	2.70459800
C	3.65356200	-1.44823600	1.75055800
H	3.27178800	-2.39873000	2.14082100
H	4.72834200	-1.39613200	1.95661600
H	3.16630300	-0.62830000	2.28976100
C	3.91719800	0.02455900	-0.26967500
H	3.71110800	0.15320500	-1.33737800
H	3.43693600	0.84704200	0.27519600
H	4.99806700	0.09598400	-0.10492200
H	-0.90212600	-2.78103800	-0.23341800
H	-1.24340500	-2.32095000	1.48954400
C	-2.52676600	0.01262700	-1.91095800
H	-1.48591200	0.30475100	-1.72506200
H	-2.69973200	0.05125800	-2.99319000
H	-3.18935700	0.75526300	-1.44557900
C	-4.22477100	-1.84487000	-1.71082900
H	-4.40776500	-2.85860000	-1.33758700
H	-4.98035000	-1.17698900	-1.27743600
H	-4.37518100	-1.84256900	-2.79638900
C	4.09365800	-2.39869300	-0.44160500

N	4.64798600	-3.26356800	-0.98598400
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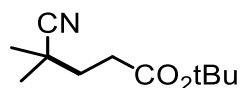
TS II_{AIBN-I₂HAT}



E = -966.4976004

G_{Corr.} = 0.440929

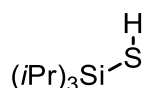
C	3.41210700	-0.51673700	0.50542500
C	2.11109500	-1.01561400	-0.18163800
H	2.21942300	-0.89045800	-1.26794200
H	2.02728600	-2.09555300	0.01402200
C	0.86008700	-0.31535600	0.26840400
H	0.63127200	-0.35070800	1.33719600
C	0.51792500	0.95134900	-0.37847000
O	0.79351900	1.22942800	-1.53793600
O	-0.18872100	1.75549700	0.44555600
C	-0.77666800	3.00609200	-0.03510300
C	0.31133300	3.95957500	-0.50408300
C	-1.80548300	2.70692400	-1.11405000
C	-1.45683300	3.56681700	1.20251200
H	1.07285000	4.07420600	0.27784200
H	0.79394900	3.60833300	-1.41869500
H	-0.13040700	4.94561000	-0.69349000
H	-2.52449000	1.96119600	-0.74898000
H	-2.35558000	3.62422900	-1.35729300
H	-1.33645800	2.32922100	-2.02709400
H	-1.91913800	4.53229000	0.96691000
H	-2.23963600	2.88938700	1.56294600
H	-0.72810800	3.71831400	2.00723900
N	-2.31247900	-1.24131900	-0.28918500
C	-3.47006100	-1.04226400	-1.13848800
H	-4.22313200	-0.45365100	-0.60436300
H	-3.20772500	-0.48046700	-2.04020000
H	-3.94285400	-1.99128600	-1.45185100
C	-1.14117700	-1.83145700	-0.82686200
C	-0.92096900	-1.56392700	-2.29459000
C	-0.84712900	-3.27351900	-0.45137700
H	-0.16464500	-1.14045800	-0.25609800
H	-1.00783700	-0.49768300	-2.53379600
H	0.08895100	-1.88310300	-2.57666400
H	-1.62898800	-2.12691300	-2.92189500
H	-0.82506800	-3.44516200	0.63048900
H	-1.61686900	-3.93483000	-0.88238900
H	0.12169400	-3.58439800	-0.85965300
C	-2.57086900	-1.41995000	1.14287700
C	-3.61492300	-2.49164300	1.44457400
C	-2.92618200	-0.09184100	1.79804200
H	-1.61463900	-1.74105800	1.58002400
H	-3.37525100	-3.44222000	0.95361600
H	-3.67435300	-2.66998000	2.52469700
H	-4.61266200	-2.17989800	1.10965900
H	-2.12208600	0.63419700	1.62986200
H	-3.85956600	0.32441400	1.39508600
H	-3.06622100	-0.22239300	2.87808000
C	3.39108400	-0.79420600	2.01250400
H	3.19705000	-1.85300400	2.21956200
H	4.34762200	-0.52131200	2.47157500
H	2.60629400	-0.19527200	2.48776300
C	3.66358700	0.97204600	0.24288000
H	3.67088500	1.19376900	-0.82951400
H	2.87113600	1.56798700	0.71313100
H	4.62111300	1.28323900	0.67495500
C	4.52010200	-1.28456600	-0.08315400
N	5.38757000	-1.90101500	-0.55111600

P_{AIBN}

E = -635.5980074

G_{Corr.} = 0.240686

C	-2.46022800	0.31618700	-0.06927500
C	-1.84573200	-0.94286000	-0.72328500
H	-1.76689600	-1.73847500	0.02909200
H	-2.54407600	-1.29920200	-1.49129500
C	0.65766200	-0.77559600	-0.35066400
O	0.69194200	-1.53970200	0.59137200
O	1.61034500	0.10609100	-0.66473100
C	2.83798500	0.24383700	0.13694600
C	2.48272100	0.70866800	1.53839700
C	3.61846300	-1.05875900	0.13048700
C	3.60076700	1.32500300	-0.60647300
H	1.88553100	1.62794000	1.49563900
H	1.92784100	-0.05328200	2.09223900
H	3.40606500	0.93205000	2.08604800
H	3.78169300	-1.39975300	-0.89880400
H	4.59969900	-0.88725200	0.58902700
H	3.10639900	-1.84509700	0.69006100
H	4.54693000	1.53147200	-0.09373600
H	3.82329700	1.00707800	-1.63135100
H	3.01805100	2.25225700	-0.64690000
C	-1.54624600	0.92281300	1.00238600
H	-1.25997900	0.18106600	1.75582000
H	-0.63472300	1.31557800	0.53402100
H	-2.04489600	1.75884700	1.50471400
C	-2.82404400	1.37772600	-1.11526900
H	-3.33634000	2.22435800	-0.64538600
H	-1.91724800	1.76203000	-1.59496300
H	-3.47949500	0.96375200	-1.88965000
C	-3.70810000	-0.11359900	0.58226300
N	-4.69658000	-0.45141500	1.09160500
C	-0.47362900	-0.72868100	-1.35014000
H	-0.27844100	-1.54802200	-2.05532000
H	-0.41336600	0.19500300	-1.93585200

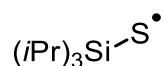
(iPr)₃SiSH

E = -1043.769941

G_{Corr.} = 0.2466

Si	0.03299000	0.05028300	0.15902500
S	-0.75725400	0.42367700	2.17464300
H	-0.14963000	-0.64987800	2.72587100
C	1.79729200	0.76492700	0.10602700
C	2.30493700	1.08740300	-1.30003700
C	2.79608400	-0.11781000	0.85259600
H	1.70981600	1.71426600	0.66100800
H	1.65201700	1.78900000	-1.83373600
H	3.30456000	1.54207500	-1.25382000
H	2.39484900	0.18480800	-1.91991600
H	2.46491100	-0.35402900	1.87277300
H	2.95991000	-1.06883000	0.32626400
H	3.77375300	0.37707300	0.93270900
C	0.04154000	-1.82848100	-0.13150700
C	0.44434200	-2.15388500	-1.57242200
C	-1.24870600	-2.55696000	0.24056100
H	0.83795600	-2.20107100	0.53647900
H	1.42481700	-1.74170000	-1.84148000
H	0.49441800	-3.24081600	-1.72652600

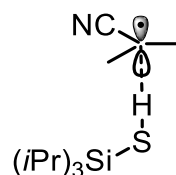
H	-0.28870700	-1.76100000	-2.29134400
H	-1.56524400	-2.35213000	1.26987800
H	-2.07828100	-2.27059500	-0.41835400
H	-1.11665700	-3.64324500	0.13914200
C	-1.08781400	1.04051600	-1.00562600
C	-1.12102100	2.51607400	-0.60091000
C	-2.50726100	0.48996200	-1.12821300
H	-0.60335300	0.96679000	-1.99523100
H	-0.12030900	2.95804200	-0.51432500
H	-1.68177200	3.10887500	-1.33660500
H	-1.62414200	2.64739400	0.36743300
H	-2.52979900	-0.51187600	-1.57320400
H	-2.99949900	0.42973000	-0.14746400
H	-3.12175100	1.14385600	-1.76301200

(iPr)₃SiS·

E = -1043.125448

G_{Corr.} = 0.23825

Si	0.04995300	0.04702300	0.17928100
S	-0.55803900	0.12612900	2.25805600
C	1.90691600	0.48126800	0.13983400
C	2.39711700	0.89576400	-1.24882600
C	2.76819600	-0.64773800	0.70178900
H	2.00720700	1.35183300	0.80980300
H	1.85359700	1.75794100	-1.65336200
H	3.46161400	1.16662900	-1.21363600
H	2.30131300	0.07504000	-1.97324000
H	2.42271000	-0.98464900	1.68726100
H	2.76703000	-1.51809200	0.03019600
H	3.81318100	-0.32516000	0.80637500
C	-0.26295200	-1.76685400	-0.32486800
C	-0.12674000	-1.93703000	-1.83854100
C	-1.58394100	-2.34973800	0.17600900
H	0.55421800	-2.32273400	0.16287500
H	0.84514400	-1.59506300	-2.21723300
H	-0.23182200	-2.99491600	-2.11789700
H	-0.90662000	-1.38262200	-2.37883500
H	-1.65954600	-2.32235800	1.27108900
H	-2.45044400	-1.80953800	-0.22645200
H	-1.68189300	-3.39898300	-0.13606300
C	-0.93597900	1.31279100	-0.83209600
C	-0.71218000	2.72320400	-0.28423800
C	-2.42961400	1.00240700	-0.90081300
H	-0.52275600	1.26516300	-1.85495100
H	0.34790800	3.00550100	-0.25041100
H	-1.23261400	3.46975300	-0.89996300
H	-1.11043600	2.80979200	0.73688000
H	-2.63935300	0.05707500	-1.41617500
H	-2.86744700	0.93925700	0.10567200
H	-2.96664800	1.79529800	-1.44024200

TS I_{AIBN}-RSH_{HAT}

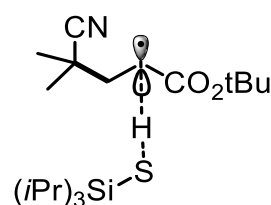
E = -1254.399538

G_{Corr.} = 0.322625

C	3.59663300	-1.70492800	-0.56054200
H	3.53256200	-1.72941100	-1.65278600
H	4.64244600	-1.87758600	-0.27175100

H	2.99071800	-2.52234900	-0.15372600
C	2.99574100	-0.29252800	1.49447200
H	2.62438800	0.68572700	1.81626200
H	2.32748300	-1.07567500	1.87164100
H	3.98216400	-0.44787500	1.95462900
C	3.62791300	0.77782000	-0.65376800
N	4.00769600	1.73965100	-1.19387300
C	3.11869900	-0.38977800	-0.00269400
H	1.76928500	-0.39025300	-0.49958500
Si	-1.05858100	0.06509200	0.01578500
S	0.50252100	-0.58491500	-1.36796000
C	-0.32379000	1.37030400	1.18582800
C	-1.36578600	1.89516800	2.17622800
C	0.34749000	2.53082400	0.45481100
H	0.44623100	0.83377600	1.76476100
H	-1.86715500	1.09391100	2.73478800
H	-0.89829200	2.56514800	2.91103600
H	-2.14074800	2.47974500	1.66077800
H	1.12202300	2.20025000	-0.24850100
H	-0.38492100	3.11308500	-0.12176100
H	0.81650200	3.22230800	1.16919500
C	-2.43497000	0.80598400	-1.07444900
C	-3.78715700	0.79855700	-0.35594700
C	-2.56658200	0.16517200	-2.45621100
H	-2.12915800	1.85659200	-1.21999500
H	-3.74986300	1.25925400	0.63897400
H	-4.53727900	1.34607500	-0.94330400
H	-4.16481900	-0.22541100	-0.22986800
H	-1.64555300	0.25432900	-3.04416500
H	-2.81209000	-0.90353100	-2.38527900
H	-3.37336100	0.64542800	-3.02756600
C	-1.66329500	-1.43663700	1.01112100
C	-0.56966400	-1.98943300	1.92302200
C	-2.21362000	-2.54481200	0.11411900
H	-2.48621000	-1.06303000	1.64511100
H	-0.20279600	-1.24676300	2.64388200
H	-0.93614800	-2.85134500	2.49790100
H	0.28898800	-2.34037500	1.32985800
H	-3.06783800	-2.21361700	-0.48969800
H	-1.44113900	-2.91028200	-0.57707000
H	-2.54917100	-3.40260700	0.71377400

TS II_{AIBN}-RSH_{HAT}



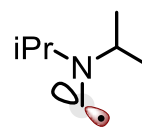
$$E = -1678.708917$$

$$G_{\text{Corr.}} = 0.493034$$

C	3.06590600	-2.37696300	0.33015500
C	1.92469100	-1.76172800	-0.52825400
H	2.27838200	-1.62072700	-1.55778200
H	1.09655900	-2.48522200	-0.56355100
C	1.44310200	-0.44803200	-0.00579700
H	1.07049500	-0.39039800	1.02014400
C	2.07318900	0.78730000	-0.52263100
O	2.68666700	0.83388300	-1.57250200
O	1.84607300	1.81535800	0.29974800
C	2.37021900	3.15982900	0.00257400
C	3.88855500	3.11768100	-0.03818500
C	1.76029000	3.67802500	-1.28816900
C	1.89477700	3.97632400	1.18980900
H	4.28046900	2.66446800	0.88082500
H	4.25954800	2.55683300	-0.89966500
H	4.27256300	4.14285200	-0.09997400
H	0.66568100	3.61664800	-1.24602800
H	2.03553000	4.73202700	-1.41417300

H	2.11268200	3.11967500	-2.15890100
H	2.23631600	5.01235200	1.08656900
H	0.80044400	3.97620900	1.24864200
H	2.29639400	3.56961100	2.12493000
H	0.13833400	-0.29841100	-0.70728600
S	-1.06379100	-0.17956900	-1.59810800
Si	-2.53804700	-0.13010400	0.01511400
C	-1.95636200	1.13655500	1.30954100
C	-4.16248100	0.42482300	-0.81234000
C	-2.68758900	-1.85001100	0.80936500
C	-2.91469300	1.21243100	2.50014300
C	-1.73288100	2.52447000	0.71573000
H	-0.98227400	0.76782700	1.67574000
C	-5.38367600	0.00062000	0.00836100
C	-4.32082500	-0.02060300	-2.26619100
H	-4.11145500	1.52713600	-0.80353800
C	-1.42574800	-2.24356600	1.57509400
C	-3.04731600	-2.93458900	-0.20478700
H	-3.51649700	-1.76246700	1.53334700
H	-3.10737600	0.23416200	2.95934300
H	-2.51107300	1.86958900	3.28279300
H	-3.88348000	1.63564300	2.19879500
H	-0.97590800	2.51120300	-0.07875600
H	-2.65941900	2.93570300	0.29062700
H	-1.39798700	3.22765500	1.49221900
H	-5.32488400	0.30967800	1.05951300
H	-6.29955600	0.43882300	-0.41166900
H	-5.51472400	-1.09005500	-0.00689300
H	-3.52027400	0.36361000	-2.90975400
H	-4.32015200	-1.11540900	-2.35729300
H	-5.27517800	0.33870600	-2.67606300
H	-1.15311000	-1.52209100	2.35669100
H	-1.54851300	-3.22259300	2.05901400
H	-0.57068500	-2.33520600	0.88916200
H	-3.99421400	-2.73299000	-0.72097700
H	-2.26648900	-3.02676600	-0.97277000
H	-3.14337100	-3.91285300	0.28663500
C	2.56066300	-2.79668500	1.71528300
H	2.22978800	-1.91638700	2.27837400
H	1.72156800	-3.49759900	1.63860200
H	3.36121500	-3.27843500	2.28679500
C	4.25457800	-1.41786600	0.45940400
H	4.60635100	-1.08163900	-0.52167200
H	3.95763700	-0.53653300	1.04297300
H	5.08440600	-1.90241700	0.98475600
C	3.51869900	-3.58611700	-0.37402400
N	3.87500900	-4.54470800	-0.92572400

I₁



$$E = -330.9147445$$

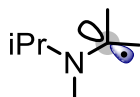
$$G_{\text{Corr.}} = 0.181814$$

$$H_{\text{Corr.}} = 0.229483$$

N	-0.00329100	-0.02526600	0.60616200
C	-0.38031000	-0.72650500	1.73450600
H	0.34202200	-0.77248800	2.54550300
H	-1.43760300	-0.297363500	1.98198700
C	-0.98558000	0.18542300	-0.46127700
C	-1.95972800	1.29401500	-0.08094000
C	-1.72225700	-1.09022800	-0.86081200
H	-0.41779800	0.52678800	-1.33757500
H	-1.42310200	2.22438600	0.13829400
H	-2.66955800	1.48313900	-0.89521400
H	-2.53739600	1.01724400	0.81018200
H	-1.02073100	-1.89731000	-1.09993800
H	-2.37802200	-1.44147200	-0.05513500

H	-2.34732400	-0.90135100	-1.74168600
C	1.42185000	0.01874000	0.27326100
C	1.83774600	1.38638800	-0.24975800
C	1.83526600	-1.10315300	-0.67387800
H	1.93966300	-0.14023200	1.23041200
H	1.54381300	2.17809000	0.44856100
H	2.92578800	1.42406300	-0.37882700
H	1.38883700	1.60699500	-1.22673400
H	1.53269300	-2.07740400	-0.27172800
H	1.37680200	-0.97878800	-1.66414800
H	2.92303400	-1.10923800	-0.81371200

I₂



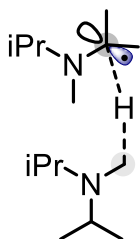
$$E = -330.9165137$$

$$G_{\text{Corr.}} = 0.182447$$

$$H_{\text{Corr.}} = 0.230161$$

N	-0.05519800	0.38671900	-0.27843000
C	0.09915000	1.76539500	0.15530400
H	1.06304500	2.15656000	-0.17888100
H	-0.67438000	2.39655300	-0.29083200
H	0.04173200	1.87916600	1.25330900
C	-1.28020000	-0.22794100	0.04823700
C	-2.49262800	0.64257300	0.09647300
C	-1.47000800	-1.65597300	-0.35064600
H	-2.71498800	1.11629900	-0.88077700
H	-3.36929900	0.04558300	0.36729600
H	-2.41903600	1.45722300	0.82794400
H	-1.29544200	-1.81994400	-1.43149300
H	-0.81353500	-2.35931100	0.18117300
H	-2.49893000	-1.96470500	-0.14040100
C	1.15776500	-0.43828900	-0.13536900
C	1.54563300	-0.65889800	1.32374400
C	2.32563600	0.11002000	-0.94228000
H	0.90857200	-1.41094800	-0.57618200
H	0.69612500	-1.04663400	1.90022400
H	2.37377400	-1.37357800	1.40103100
H	1.87348100	0.27922800	1.79097700
H	2.01462600	0.36443300	-1.96191800
H	2.77364800	0.99983500	-0.48268600
H	3.11490600	-0.64811300	-1.00255800

TS I₁-I₂



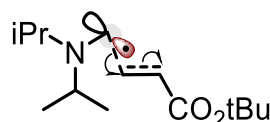
$$E = -662.4573924$$

$$G_{\text{Corr.}} = 0.394573$$

N	-2.52781100	0.25128700	0.56081200
C	-2.19302400	-0.85408100	1.44516400
H	-3.06278400	-1.49842900	1.59619500
H	-1.36423900	-1.47853800	1.06102300
H	-1.89846800	-0.48308700	2.43175400
C	-1.39378400	1.08862600	0.25289000
C	-0.70622100	1.61847400	1.49226700
C	-1.66937500	2.18718800	-0.74610600

H	-0.40577400	0.33869600	-0.33693100
H	-0.23130900	0.83173300	2.09053200
H	0.08860200	2.31795700	1.20594400
H	-1.41744200	2.15913200	2.13944000
H	-1.91158300	1.81396000	-1.74898800
H	-2.49538600	2.84105500	-0.41938200
H	-0.77482300	2.81300100	-0.84879500
C	-3.39601500	-0.12365900	-0.56733800
C	-4.73362000	-0.67467400	-0.08976400
C	-2.74530500	-1.07759800	-1.56737800
H	-3.62509700	0.81347600	-1.08992200
H	-5.15315200	-0.04893700	0.70613800
H	-5.44255000	-0.69068500	-0.92575600
H	-4.65689800	-1.70429400	0.28184000
H	-1.82300700	-0.65948900	-1.98790100
H	-2.49726800	-2.03754000	-1.09431800
H	-3.43217800	-1.28646200	-2.39696000
C	0.68029000	-0.35607500	-0.88569000
N	1.82998300	-0.13888600	-0.09253300
H	0.73351700	0.03454800	-1.91796500
H	0.34511100	-1.39735200	-0.88106200
C	2.50499400	1.13897600	-0.29850300
C	2.61154200	-1.29356700	0.35554400
C	3.52265900	1.12074400	-1.43867500
C	3.13076800	1.67390900	0.98342800
H	1.69788200	1.83589400	-0.57953600
C	3.01260100	-2.25112800	-0.76691000
C	1.87832200	-2.03594300	1.46670100
H	3.53630800	-0.88626600	0.78871500
H	3.07628200	0.73456800	-2.36354800
H	3.90153400	2.13068600	-1.63930200
H	4.38474300	0.48934000	-1.18384800
H	2.40607000	1.66130000	1.80634700
H	4.00631500	1.08680800	1.28933300
H	3.47283800	2.70537100	0.83555900
H	3.52224500	-1.72533200	-1.58232300
H	3.68765300	-3.02673000	-0.38434300
H	2.13516400	-2.75743100	-1.18939500
H	1.65629000	-1.35959400	2.30131900
H	0.92627000	-2.44624800	1.10186900
H	2.47695200	-2.87508100	1.84252500

TS I₁-II₁



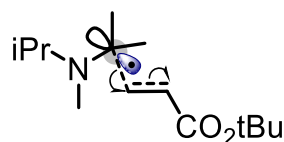
$$E = -755.1912092$$

$$G_{\text{Corr.}} = 0.345368$$

C	-2.66806400	2.54434400	-0.46621700
C	-2.89849500	1.29457400	0.37384800
H	-3.92310400	1.33878500	0.76679500
H	-3.38077600	2.59362000	-1.29767800
H	-2.78535000	3.44476200	0.14776000
H	-1.65348300	2.55647900	-0.88371200
C	-1.94447000	1.23325400	1.56196700
H	-2.14440800	0.35553500	2.18796900
H	-0.89629900	1.19047500	1.23843300
H	-2.06665400	2.12816600	2.18338400
N	-2.84069700	0.08901600	-0.46365700
C	-3.97958300	-0.83271800	-0.47647000
C	-5.23680000	-0.16670300	-1.01743200
C	-4.21200500	-1.47203300	0.88762600
H	-3.69260600	-1.62877500	-1.17860100
H	-5.05329100	0.27283600	-2.00415100
H	-6.04194500	-0.90457200	-1.11115900
H	-5.59885500	0.62579900	-0.35017700
H	-3.30005000	-1.96162600	1.24891300
H	-4.52067200	-0.72580400	1.63149000
H	-5.00733600	-2.22435000	0.82668400
C	-1.64575700	-0.33045100	-0.97012200

H	-1.67225900	-1.10837400	-1.72864000
H	-0.82636900	0.38225500	-0.99832100
C	-0.13269700	-1.83770900	0.48265000
H	-0.44170300	-1.12872700	1.24585900
H	-0.78430600	-2.68679000	0.29518700
C	1.10890500	-1.76963100	-0.05245400
H	1.47848700	-2.51582200	-0.75186500
C	1.98110600	-0.63936700	0.24783400
O	1.66889400	0.32669000	0.93136300
O	3.18681700	-0.79353000	-0.34119900
C	4.24812800	0.19954600	-0.20356300
C	3.81384200	1.52538700	-0.80756100
C	4.66120100	0.33449300	1.25319200
C	5.38105100	-0.40236300	-1.01748300
H	3.46515400	1.37678700	-1.83677100
H	3.01575000	1.99212100	-0.22523600
H	4.67259800	2.20742000	-0.83512500
H	4.91054300	-0.64926000	1.66887400
H	5.55526300	0.96691100	1.31688700
H	3.87010400	0.78524400	1.85733700
H	6.25410900	0.25992400	-0.99179600
H	5.67177700	-1.37790900	-0.61111600
H	5.07669500	-0.53724400	-2.06182200

TS I₂-II₂



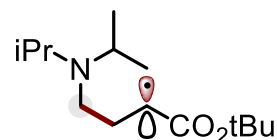
$$E = -755.1957426$$

$$G_{\text{Corr.}} = 0.34776$$

N	2.74557800	0.16570900	0.12164700
C	1.98792400	1.43139300	0.16653100
C	1.80465500	2.06234400	-1.20800900
C	2.63456700	2.40066500	1.14720200
H	0.98369700	1.18329400	0.52503700
H	1.35432600	1.35550200	-1.91260600
H	1.11715500	2.91135400	-1.12026200
H	2.74630000	2.44200200	-1.62350300
H	2.69481700	1.96472600	2.15087600
H	3.65206500	2.66643400	0.83050000
H	2.05413800	3.32924900	1.20667100
C	2.18972800	-1.02441500	0.54479400
C	0.71780600	-1.75225200	-1.23739400
H	1.06598800	-0.86643200	-1.76511900
H	1.28954800	-2.66615200	-1.37573700
C	-0.56634500	-1.80366600	-0.77515500
H	-0.98404500	-2.71577600	-0.35344000
C	-1.37532400	-0.60315300	-0.69553800
O	-1.03598300	0.50710400	-1.09319600
O	-2.56698700	-0.85503700	-0.09746000
C	-3.50223000	0.21637500	0.21876300
C	-2.85768500	1.20389100	1.18050200
C	-4.00451300	0.88624000	-1.05074800
C	-4.64095800	-0.51734400	0.90735000
H	-2.47297800	0.67485800	2.06181100
H	-2.03752400	1.75129700	0.70698200
H	-3.61075700	1.92559100	1.52032800
H	-4.39833600	0.13301200	-1.74383100
H	-4.82060800	1.57457700	-0.79777000
H	-3.21231200	1.44780000	-1.55118600
H	-5.42112800	0.19325100	1.20425400
H	-5.08422200	-1.25899300	0.23280500
H	-4.28072600	-1.03473700	1.80405800
C	3.92520200	0.15367400	-0.72110000
H	3.70555100	-0.17286100	-1.75163200
H	4.35019800	1.15959600	-0.77076500
H	4.69815100	-0.50003100	-0.30859900
C	1.19282200	-0.97118900	1.65998000
H	0.26747300	-0.44040300	1.40172300

H	0.89957800	-1.98737400	1.94098300
H	1.62092100	-0.48081200	2.54913300
C	3.07757400	-2.23082800	0.52927800
H	3.89552900	-2.13881000	1.26576900
H	2.49573600	-3.11847700	0.79664600
H	3.53685600	-2.41860800	-0.44814600

II₁

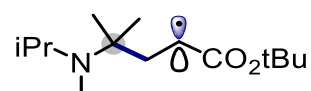


$$E = -755.2202148$$

$$G_{\text{Corr.}} = 0.349125$$

C	4.32196800	-1.06716100	1.44898300
C	3.62280300	-1.12702500	0.09050100
H	3.04012600	-2.06197400	0.06526700
H	3.59820500	-1.00987400	2.27171700
H	4.93750400	-1.96195600	1.60411500
H	4.98706600	-0.19578900	1.51504300
C	4.63639400	-1.20948800	-1.04330900
H	4.12599000	-1.29723600	-2.00937800
H	5.27948800	-0.32027300	-1.07798700
H	5.29293700	-2.07826800	-0.91220400
N	2.64582800	-0.06400900	-0.14279700
C	3.09816600	1.32690900	-0.07157500
C	2.91637500	2.00541500	1.28898900
C	2.43328900	2.14731200	-1.17076600
H	4.17715300	1.30310100	-0.28417600
H	3.33982800	1.40946500	2.10477300
H	3.41192000	2.98420200	1.29084400
H	1.85652900	2.18281500	1.51332300
H	2.65582700	1.72122700	-2.15603300
H	1.34113100	2.15545800	-1.04677400
H	2.77627300	3.18937800	-1.15060600
C	1.31399200	-0.34475200	0.33582300
H	1.32272900	-0.90624600	1.29004500
H	0.78215900	0.59285200	0.53930900
C	0.47980000	-1.12677500	-0.70874100
H	0.44733900	-0.50640700	-1.61464600
H	0.99861600	-0.83032800	-0.95199400
C	-0.88792100	-1.40108100	-0.22590300
H	-1.13257500	-2.31969900	0.30443900
C	-1.92113600	-0.38921200	-0.34043800
O	-1.74632200	0.70887300	-0.85419100
O	-3.08397100	-0.81410000	0.19120200
C	-4.28150300	0.02832000	0.19936200
C	-4.03108900	1.28848000	1.01146100
C	-4.71753800	0.33161200	-1.22456500
C	-5.30727700	-0.85228500	0.89086300
H	-3.65974400	1.02908300	2.01017900
H	-3.31002700	1.94901700	0.52337000
H	-4.97667300	1.83107100	1.13145900
H	-4.82691700	-0.59876700	-1.79459600
H	-5.69304900	0.83241000	-1.20180700
H	-4.00494900	0.98218500	-1.73756200
H	-6.26590900	-0.32555500	0.95946800
H	-5.46016200	-1.78107800	0.32948200
H	-4.97719500	-1.10759400	1.90430300

II₂

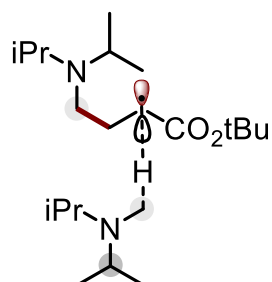


$$E = -755.2202026$$

$G_{\text{Corr.}} = 0.349915$

N	-2.93918200	-0.41215300	0.39310700
C	-4.08627200	0.38381700	-0.07267500
C	-5.39704300	-0.33748200	0.22654400
C	-4.05501500	0.80243100	-1.54569700
H	-4.09830200	1.29650400	0.53484500
H	-5.40305900	-0.73462500	1.24807600
H	-6.23314600	0.36362500	0.12381000
H	-5.58370500	-1.16507600	-0.46959100
H	-3.24443400	1.50570800	-1.76661100
H	-3.94285600	-0.06565700	-2.20837000
H	-4.99712900	1.29730500	-1.81273100
C	-1.63055800	0.23443400	0.58874500
C	-0.77171800	0.23124800	-0.73431100
H	-0.68325500	-0.80359000	-1.08672200
H	-1.32694700	0.80632300	-1.48739500
C	0.57852500	0.79487400	-0.57501200
H	0.73615700	1.87097200	-0.51724400
C	1.74527800	-0.05729200	-0.45128400
O	1.72112700	-1.27884200	-0.53233100
O	2.85719700	0.67427400	-0.23041900
C	4.15820500	0.04338000	-0.00647100
C	4.10366800	-0.83655900	1.23215000
C	4.59332800	-0.72168000	-1.24557300
C	5.07314900	1.23237000	0.22900000
H	3.71646100	-0.26583700	2.08534900
H	3.47357800	-1.71618900	1.07763300
H	5.11797500	-1.17206000	1.48019300
H	4.56114600	-0.06813800	-2.12558300
H	5.62773300	-1.06146300	-1.11268000
H	3.96037600	-1.59390700	-1.42632700
H	6.09701500	0.88596500	0.41026900
H	5.07947600	1.89366300	-0.64503800
H	4.74140300	1.80896600	1.10007400
C	-2.89313900	-1.74811800	-0.17272500
H	-2.04082500	-2.30478700	0.22390600
H	-3.79062500	-2.31101400	0.10461900
H	-2.81340700	-1.76934200	-1.27537500
C	-0.86718700	-0.52255900	1.68119500
H	-0.60709100	-1.54595500	1.39257800
H	0.07516400	-0.00911300	1.91366300
H	-1.47524300	-0.55994500	2.59255900
C	-1.80190600	1.67136200	1.07368800
H	-2.45128800	1.70442800	1.95725300
H	-0.82697500	2.07627400	1.36623800
H	-2.21642100	2.33723600	0.30739600

TS II₁-I₁



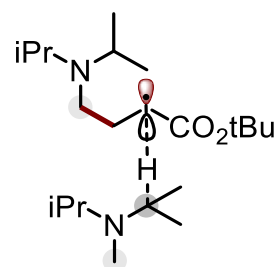
$E = -1086.774624$

$G_{\text{Corr.}} = 0.56314$

C	-4.48661400	0.23573900	0.82282500
N	-3.89313000	-0.17282300	-0.44696000
C	-4.31623500	-1.43049300	-1.04808300
C	-5.75741700	-1.34993500	-1.54573600
C	-4.12756100	-2.66200700	-0.15852600
H	-3.67461200	-1.55914400	-1.93526400
H	-5.88190600	-0.50482100	-2.23221900
H	-6.04502100	-2.27146800	-2.06745000
H	-6.46005600	-1.21425200	-0.71237300

H	-3.08930800	-2.76325400	0.17777800
H	-4.76694700	-2.60466200	0.73301000
H	-4.40363800	-3.57657000	-0.69894300
C	-2.58786500	0.33151500	-0.80421400
C	-1.36687800	-0.52721600	-0.43108000
H	-1.35806500	-0.71778900	0.65120900
H	-1.44739700	-1.50555900	-0.93079200
C	-0.07208900	0.12410800	-0.83392700
H	0.07308900	0.26713800	-1.90981500
C	0.36113800	1.26584300	-0.03615800
O	-0.01043800	1.50964900	1.10594900
O	1.27581500	2.01418400	-0.70440400
C	1.84883000	3.22818100	-0.13319500
C	0.75523000	4.25001200	0.13649200
C	2.65719800	2.91069300	1.11500000
C	2.76650900	3.72290400	-1.23916700
H	0.15516600	4.40899900	-0.76778400
H	0.09664300	3.93060100	0.94794100
H	1.21416600	5.20732300	0.41274500
H	3.41523100	2.14788800	0.89422700
H	3.17882500	3.81723200	1.44635500
H	2.01976500	2.55621600	1.92933400
H	3.26266700	4.64975400	-0.92849200
H	3.53708900	2.97652400	-1.46702900
H	2.19547100	3.92301600	-2.15311800
N	2.76885100	-2.14776100	-0.18791100
C	3.10643600	-2.03036300	1.23703100
H	4.16939700	-1.75684200	1.27846000
C	1.42441000	-2.14244700	-0.55099800
H	0.85139000	-0.92032300	-0.62154200
C	3.74002300	-1.69568700	-1.18779900
C	5.02936200	-2.50182000	-1.11836800
C	4.00283900	-0.19467900	-1.11838800
H	3.26660900	-1.91028300	-2.15775100
H	4.82361200	-3.57645700	-1.17759800
H	5.68702500	-2.22786400	-1.95132500
H	5.58425000	-2.30878500	-0.19141000
H	3.06925200	0.37800000	-1.19026600
H	4.50221400	0.07608700	-0.17717400
H	4.66065000	0.11632400	-1.93953800
H	-5.35896300	-0.41786800	0.97326200
H	0.77076800	-2.63976700	0.17438200
H	1.25354600	-2.50959600	-1.56973200
C	2.94594400	-3.37700300	1.93154400
H	3.56678600	-4.14072200	1.44932800
H	3.23625100	-3.30523700	2.98648400
H	1.90185200	-3.71438100	1.89679200
C	2.31928700	-0.93674600	1.94971200
H	2.42973900	0.03297600	1.45140600
H	1.24732500	-1.16866800	1.99101800
H	2.67373200	-0.83175400	2.98179700
C	-3.57953300	0.06491300	2.04207600
H	-2.68988300	0.70500700	1.97153200
H	-4.11646100	0.34697000	2.95679800
H	-3.24417900	-0.97328400	2.15220100
C	-5.01371500	1.66612100	0.74342700
H	-5.72515200	1.76617700	-0.08495400
H	-5.51633600	1.95474700	1.67542400
H	-4.19604400	2.38025500	0.57722400
H	-2.46341100	1.32537300	-0.35070800
H	-2.55398400	0.49635900	-1.89648400

TS II₁-I₂

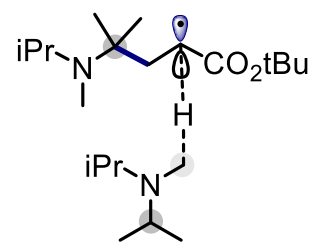


E = -1086.773119

G_{Corr.} = 0.563542

C	4.91553700	-2.10327000	-0.22837900
C	4.53119400	-0.76743100	0.40208700
H	5.46919100	-0.23656500	0.62350400
H	5.49732600	-1.94127700	-1.14356200
H	5.51171600	-2.71059100	0.46452100
H	4.02345800	-2.68718400	-0.49174900
C	3.81283300	-0.98952600	1.73371400
H	3.58773200	-0.03978400	2.23343600
H	2.86908400	-1.53342000	1.59270700
H	4.43972200	-1.58722200	2.40764400
N	3.81149400	0.07101300	-0.55280000
C	4.25290900	1.44513800	-0.75337900
C	5.60523100	1.49417400	-1.46023700
C	4.28290800	2.30230100	0.51490000
H	3.51354500	1.89061000	-1.43911900
H	5.56980200	0.93106800	-2.39973800
H	5.89537600	2.52896400	-1.68161600
H	6.39771500	1.05983300	-0.83584000
H	3.30857200	2.31910800	1.01733300
H	5.02469100	1.92069500	1.22970600
H	4.56274000	3.33644400	0.27645700
C	2.43158400	-0.23370800	-0.84774800
H	2.23378200	-0.00780800	-1.91111500
H	2.28339800	-1.31763600	-0.74109000
C	1.35297700	0.48708300	-0.01664000
H	1.51161100	0.28894900	1.05224000
H	1.45237300	1.57303700	-0.16485400
C	-0.03373900	0.06573000	-0.40781900
H	-0.35348800	0.32873500	-1.42177300
C	-0.49163100	-1.25217900	0.02606500
O	0.03266600	-1.92346500	0.90618100
O	-1.62636700	-1.60504600	-0.62121700
C	-2.37983000	-2.80179700	-0.26155000
C	-1.55739400	-4.04769700	-0.54808800
C	-2.83812200	-2.72955100	1.18658500
C	-3.58413000	-2.73712100	-1.18567700
H	-1.21315400	-4.04198800	-1.58936400
H	-0.68941900	-4.11555100	0.11250800
H	-2.18184300	-4.93754700	-0.40093800
H	-3.38111800	-1.79068000	1.36135300
H	-3.52680600	-3.55916500	1.38872200
H	-1.99918300	-2.79371200	1.88429200
H	-4.22304700	-3.61434700	-1.03108600
H	-4.17523700	-1.83478200	-0.98362500
H	-3.26642400	-2.71708400	-2.23501400
N	-2.97530900	1.49945000	0.34139900
C	-4.21832700	1.41070700	1.07754500
H	-5.03107400	1.12423700	0.40076200
H	-4.16379100	0.63932300	1.85232700
H	-4.50415000	2.36086300	1.56704800
C	-1.74677300	1.62610200	1.03858800
C	-1.70155200	0.92914600	2.37415700
C	-1.10175500	2.99965800	1.07758700
H	-0.89930600	0.89367500	0.31732000
H	-2.06046000	-0.10552500	2.30775100
H	-0.66616700	0.89817800	2.73376900
H	-2.29726900	1.45413400	3.13676800
H	-0.97530000	3.44292000	0.08320800
H	-1.71873600	3.68927200	1.67780800
H	-0.11131400	2.94364200	1.54623400
C	-3.04548500	2.05256700	-1.01321500
C	-3.78506500	3.38585200	-1.08887800
C	-3.62635100	1.03610300	-1.98865700
H	-2.00308500	2.22503600	-1.31768600
H	-3.38426100	4.11230900	-0.37174700
H	-3.69715300	3.81328400	-2.09473200
H	-4.85539600	3.25950400	-0.88018300
H	-3.04082300	0.10866900	-1.96617700
H	-4.66888800	0.79207700	-1.74277500
H	-3.61873200	1.43845800	-3.00931000

TS II₂-I₁



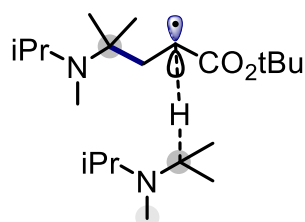
E = -1086.773998

G_{Corr.} = 0.563736

C	4.25575300	0.32164100	-1.53343100
H	3.43893300	-0.01753100	-2.19972300
N	4.07568300	-0.01698000	-0.13512100
C	4.44104300	-1.40918600	0.17976200
C	5.93911900	-1.50216500	0.44771700
C	4.01941900	-2.45846500	-0.85268200
H	3.93284600	-1.66799700	1.11688300
H	6.22289200	-0.83238000	1.26754900
H	6.23096300	-2.52663600	0.71247300
H	6.51752500	-1.21248400	-0.43998600
H	2.95242700	-2.39909500	-1.09579900
H	4.58475600	-2.36060200	-1.78812300
H	4.21930400	-3.46241800	-0.45838900
C	2.86399100	0.52875500	0.52021500
C	1.60122000	-0.29156500	0.14603600
H	1.55627600	-0.39555900	-0.94839600
H	1.72818900	-1.30457100	0.56039100
C	0.28061800	0.25791000	0.61497000
H	0.19049100	0.45307600	1.68781900
C	-0.36182900	1.26904000	-0.21552700
O	-0.24024800	1.36281900	-1.43213600
O	-1.16875300	2.07184000	0.52161900
C	-1.87972600	3.20280800	-0.06475800
C	-0.88295100	4.20231000	-0.63036300
C	-2.88486700	2.73928900	-1.10743600
C	-2.60536800	3.79904200	1.12992400
H	-0.14564300	4.47389100	0.13546000
H	-0.35784700	3.79894000	-1.50050100
H	-1.41233500	5.11450600	-0.93204600
H	-3.56171200	1.98881700	-0.67890700
H	-3.49146700	3.59618700	-1.42608300
H	-2.39129700	2.31286200	-1.98440800
H	-3.18837000	4.67345100	0.81817900
H	-3.28930700	3.06374200	1.57127600
H	-1.89002800	4.11273300	1.89885600
N	-2.35124200	-2.27569500	0.08619200
C	-2.61573800	-2.29009600	-1.35530100
H	-1.66935500	-2.61239900	-1.81411200
C	-1.03399000	-2.13931900	0.51341600
H	-0.54246700	-0.87547900	0.49783800
C	-3.43087000	-1.89490900	1.00443400
C	-3.19119800	-0.54683600	1.67595300
C	-3.67370500	-2.99419200	2.03153900
H	-4.33700700	-1.80358400	0.39030400
H	-2.97932000	0.24213100	0.94456700
H	-4.07510700	-0.25453400	2.25527100
H	-2.34122200	-0.58988100	2.36980100
H	-3.91063500	-3.94390700	1.53858000
H	-2.78616600	-3.14812400	2.65901600
H	-4.50579600	-2.72754900	2.69411600
H	4.36644500	1.40199300	-1.66609900
H	5.18412000	-0.13080400	-1.89929000
C	3.07453000	0.51819500	2.03729500
H	3.12982700	-0.49228300	2.45826700
H	4.00601900	1.04295200	2.28386900
H	2.24898800	1.03241200	2.54339000
C	2.69086400	1.99198000	0.10856800
H	2.38721400	2.10719400	-0.93755600
H	1.91460900	2.46201000	0.72529600

H	3.62662500	2.54145500	0.27229900
H	-0.31931700	-2.65772300	-0.13611300
H	-0.88290300	-2.39244400	1.56958400
C	-2.95794400	-0.91238900	-1.91035400
H	-2.15664900	-0.19170900	-1.70597700
H	-3.09600500	-0.96392800	-2.99723700
H	-3.89321200	-0.53073200	-1.47805300
C	-3.67618600	-3.32378700	-1.71102300
H	-3.40852600	-4.31137000	-1.31908500
H	-4.66209500	-3.05174600	-1.31233300
H	-3.77684600	-3.39779600	-2.79995600

TS II₂-I₂



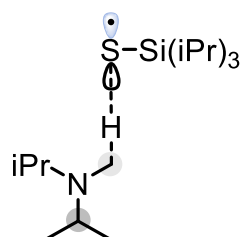
$$E = -1086.773233$$

$$G_{\text{Corr.}} = 0.564554$$

C	4.27937600	1.12658600	-1.10834700
H	3.60752700	0.85698900	-1.94623300
N	3.97226700	0.47163400	0.14841200
C	4.48002900	-0.90970700	0.22537900
C	5.93333600	-0.90121100	0.68634800
C	4.33128700	-1.74732900	-1.04833800
H	3.90143700	-1.41853300	1.00635400
H	6.02360400	-0.39747800	1.65556400
H	6.32348800	-1.92259200	0.78229600
H	6.57270400	-0.36937200	-0.03108000
H	3.30211300	-1.75666000	-1.42671800
H	4.98264200	-1.38457600	-1.85352600
H	4.62184200	-2.78455500	-0.84081300
C	2.62498700	0.72550000	0.70913300
C	1.55088600	-0.13515700	-0.00781900
H	1.65046300	0.01528800	-1.09275100
H	1.77979000	-1.19241500	0.19657300
C	0.11915900	0.12768600	0.37086500
H	-0.13220900	0.04481500	1.43275900
C	-0.58819200	1.20314400	-0.32361600
O	-0.37059900	1.54073000	-1.47993100
O	-1.55646700	1.74418800	0.45033300
C	-2.49367500	2.72789100	-0.08712900
C	-1.75303800	3.97792100	-0.53767700
C	-3.31837700	2.09715600	-1.19840000
C	-3.37645000	3.05340400	1.10628900
H	-1.09672000	4.33483300	0.26643000
H	-1.14947800	3.79361600	-1.42912700
H	-2.48003300	4.76905000	-0.75920500
H	-3.76383600	1.15702500	-0.84597500
H	-4.12993700	2.77843600	-1.48242800
H	-2.71060300	1.88914100	-2.08351300
H	-4.11803900	3.81011600	0.82528600
H	-3.90979300	2.16188900	1.45627400
H	-2.77481900	3.44729600	1.93368800
N	-2.52226000	-1.82761000	-0.30799000
C	-3.61600500	-2.12892300	-1.21019100
H	-4.56519300	-1.82799800	-0.75394800
H	-3.52102400	-1.56786000	-2.14501800
H	-3.68812300	-3.20351200	-1.46273600
C	-1.18569700	-1.98949000	-0.76186300
C	-0.97947000	-1.68448200	-2.22346400
C	-0.43805800	-3.23339900	-0.31731900
H	-0.54241600	-0.97805400	-0.16105700
H	-1.42418900	-0.72277900	-2.50537900
H	0.09477900	-1.62599000	-2.43683000
H	-1.39772600	-2.47212600	-2.86964600
H	-0.42139300	-3.36226000	0.77092200

H	-0.90666600	-4.13070500	-0.75568700
H	0.60172400	-3.20025900	-0.66591400
C	-2.77734100	-2.03690000	1.12081700
C	-3.38980300	-3.39751800	1.44435000
C	-3.61398900	-0.89884200	1.69048500
H	-1.79395200	-1.98155000	1.60964400
H	-2.80907200	-4.21988600	1.00989700
H	-3.43146100	-3.54534800	2.52996600
H	-4.41730700	-3.47214500	1.06543000
H	-3.09937300	0.05690900	1.53507100
H	-4.60157700	-0.84345900	1.21222600
H	-3.77798800	-1.04181400	2.76580000
H	4.25761700	2.21508500	-1.00064400
H	5.29953300	0.86690700	-1.41196100
C	2.64523000	0.41497100	2.20856700
H	2.79016800	-0.64944900	2.42630600
H	3.45586000	0.97580300	2.69019500
H	1.69943600	0.71324100	2.67619500
C	2.29259500	2.21187800	0.56671500
H	2.11441500	2.51060500	-0.47207000
H	1.38224700	2.44638600	1.13256300
H	3.10727900	2.82135600	0.97793300

TS RS·-I₁



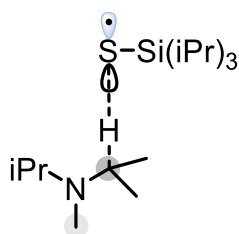
$$E = -1374.694918$$

$$G_{\text{Corr.}} = 0.447899$$

N	-3.05684200	0.15635300	-0.33327500
C	-1.93609700	0.81464000	-0.77744200
H	-1.47182900	0.38832100	-1.66911900
H	-1.97425300	1.90454500	-0.74576100
C	-3.95674400	0.81080500	0.62541600
C	-4.80137500	1.87090100	-0.07034500
C	-3.21516500	1.38074300	1.82865500
H	-4.63214600	0.02548700	0.98999600
H	-5.36546500	1.43826700	-0.90445300
H	-5.51089200	2.31862100	0.63517200
H	-4.17124500	2.67749500	-0.46603900
H	-2.60147000	0.61822700	2.32140800
H	-2.55469300	2.20755400	1.53831600
H	-3.93501500	1.77119300	2.55713500
C	-3.14754500	-1.29465500	-0.52911600
C	-4.50863600	-1.69817800	-1.07821600
C	-2.78347900	-2.07041000	0.73188200
H	-2.39449300	-1.52388700	-1.29774200
H	-4.74272900	-1.14459800	-1.99434300
H	-4.51423000	-2.76933600	-1.30991000
H	-5.31204200	-1.51886700	-0.35239200
H	-1.79641100	-1.77167700	1.10754200
H	-3.52055400	-1.90650400	1.52906500
H	-2.76302400	-3.14596100	0.51828500
Si	1.97288500	0.08648900	-0.01319600
S	0.32064100	0.37528300	1.35338400
H	-0.71296000	0.57872900	0.29266700
C	1.73462200	1.27026900	-1.48904200
C	2.84481700	1.13276500	-2.53212200
C	1.58736000	2.72916100	-1.06220000
H	0.78653100	0.95890800	-1.95997600
H	2.98071100	0.09943800	-2.87776900
H	2.63095500	1.75016600	-3.41622500
H	3.80774700	1.47819800	-2.12927500
H	0.76968900	2.87110000	-0.34487800
H	2.50735500	3.09912100	-0.58706200

H	1.39406200	3.37469000	-1.93112900
C	3.58319700	0.50003400	0.92289600
C	4.80600200	-0.16764100	0.28792300
C	3.53582400	0.19746300	2.42035600
H	3.69365200	1.59264100	0.80785400
H	4.90000300	0.03956800	-0.78552100
H	5.73122700	0.17653600	0.77146700
H	4.76926900	-1.25945100	0.40812800
H	2.72331200	0.73332200	2.92466000
H	3.38865700	-0.87492500	2.61111200
H	4.48031500	0.48594000	2.90399500
C	1.98435400	-1.71021200	-0.64598600
C	0.75391500	-2.02119500	-1.49585300
C	2.10457900	-2.72306700	0.49160800
H	2.87918700	-1.80045800	-1.28615600
H	0.66511600	-1.36540600	-2.37221600
H	0.77805200	-3.05792900	-1.86112300
H	-0.16443600	-1.90995500	-0.89914900
H	3.02157500	-2.58979800	1.07992300
H	1.25404800	-2.63569700	1.18287700
H	2.10990600	-3.75200300	0.10367900

TS RS⁻-I₂



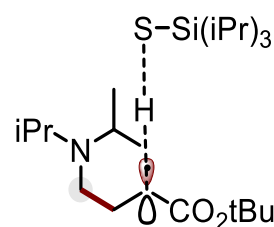
$$E = -1374.692377$$

$$G_{\text{Corr.}} = 0.446749$$

N	-3.33876800	0.25074100	0.27887700
C	-3.11074200	-0.01073000	1.69166000
H	-3.23848900	0.89577700	2.29354700
H	-3.82950400	-0.74577700	2.05824900
C	-4.14291500	-0.74204700	-0.45188300
C	-5.54728300	-0.84822000	0.13125900
C	-3.47288200	-2.10829800	-0.54120100
H	-4.25923100	-0.34798800	-1.46684600
H	-5.99963000	0.14198800	0.25363200
H	-6.17837600	-1.43479200	-0.54609900
H	-5.56121100	-1.35824000	1.10225100
H	-2.50269300	-2.04959900	-1.04740900
H	-3.30419600	-2.53317400	0.45710200
H	-4.11230900	-2.80542800	-1.09613200
C	-2.39595900	1.05219400	-0.37234900
C	-2.00837100	2.31422600	0.35448500
C	-2.54063700	1.22625600	-1.85771300
H	-1.05315800	0.20253100	-0.33742900
H	-1.69449500	2.14936300	1.38916000
H	-1.17928400	2.80686600	-0.16427200
H	-2.85818000	3.01779700	0.37146500
H	-2.47219700	0.28100900	-2.40945500
H	-3.49437700	1.71148600	-2.12327400
H	-1.73409000	1.87144000	-2.22218500
Si	1.92717400	-0.18453800	0.00243900
S	-0.04225400	-0.93264500	-0.49895500
H	-2.09875600	-0.41114400	1.86838900
C	3.04270700	-1.70165500	-0.30043700
C	4.50227400	-1.43441200	0.07162800
C	2.95608900	-2.23626000	-1.72879100
H	2.64870600	-2.47928400	0.37578200
H	4.62356500	-1.04877500	1.09246400
H	5.09890300	-2.35458700	-0.00488600
H	4.95584200	-0.70500400	-0.61493700
H	1.93046800	-2.50181000	-2.01086100
H	3.31834800	-1.49481400	-2.45573100
H	3.58153400	-3.13263000	-1.84828800

C	2.48131600	1.24939600	-1.13225000
C	3.61543900	2.07081100	-0.51348900
C	1.36041800	2.17410200	-1.59694300
H	2.87891400	0.73667400	-2.02571200
H	4.46399800	1.45593000	-0.18891000
H	3.99998900	2.80719000	-1.23349100
H	3.26465000	2.63316100	0.36328100
H	0.54309600	1.61934900	-2.07441800
H	0.93587600	2.73735200	-0.75293100
H	1.73531000	2.91366600	-2.31896900
C	2.03172000	0.30437700	1.83882400
C	1.83129300	-0.89350300	2.76525400
C	1.05241800	1.41640700	2.20425300
H	3.05731500	0.68738800	1.98072900
H	2.58716200	-1.67459500	2.61719500
H	1.87923600	-0.58510800	3.81965300
H	0.84541500	-1.35251300	2.60219200
H	1.15541200	2.30641200	1.56843000
H	0.01798100	1.05803900	2.10438900
H	1.18615800	1.73662400	3.24749500

TS II₁-P₁(RSH)



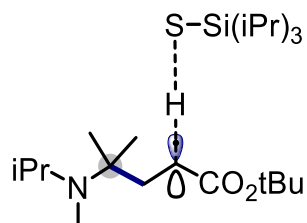
$$E = -1798.987995$$

$$G_{\text{Corr.}} = 0.61622$$

C	4.93797400	-0.90043600	-0.54300600
H	5.40306100	-1.85937100	-0.81386300
N	3.89383000	-1.22416600	0.42766000
C	3.51128500	-2.61889500	0.62273600
C	4.62857100	-3.40641000	1.30084500
C	3.04546300	-3.32874300	-0.64986100
H	2.65954900	-2.59318200	1.32237200
H	4.92144500	-2.92987600	2.24309300
H	4.30768000	-4.43382500	1.51205000
H	5.51872100	-3.46695200	0.66055500
H	2.22941200	-2.78809700	-1.14342000
H	3.86848200	-3.42970100	-1.36995400
H	2.68949800	-4.34015200	-0.41600500
C	2.94887900	-0.21620800	0.80711700
C	1.61166200	-0.21521500	0.00190900
H	1.82632900	-0.10178200	-1.06810100
H	1.12750500	-1.18929600	0.15172200
C	0.70750800	0.86673100	0.45285300
H	0.29448300	0.81061000	1.46468100
C	0.93711500	2.23654800	-0.04286900
O	1.73318500	2.51544800	-0.92329300
O	0.11389200	3.09634100	0.56718700
C	-0.05390900	4.47853100	0.10361900
C	1.22484500	5.26234500	0.34040500
C	-0.48644800	4.48729700	-1.35293200
C	-1.17420600	4.98810400	0.99208700
H	1.52919200	5.18702600	1.39113000
H	2.03953800	4.90325400	-0.29391700
H	1.04607800	6.32030300	0.11308700
H	-1.36046600	3.83889500	-1.49284200
H	-0.76960800	5.50877200	-1.63414300
H	0.31316300	4.15315700	-2.01911800
H	-1.40313700	6.03091000	0.74485500
H	-2.08011900	4.38700600	0.84701800
H	-0.88508100	4.93546700	2.04802500
H	-0.55934600	0.62275200	-0.29508600
H	2.68732900	-0.33683300	1.87151800
H	3.41484300	0.77334100	0.70925600
C	4.42931500	-0.26151900	-1.83445600

H	5.26481900	-0.09331900	-2.52505000
H	3.69596300	-0.90020400	-2.34055900
H	3.96050400	0.71304200	-1.64306600
C	6.02348300	-0.03970100	0.09642600
H	6.84340000	0.14450200	-0.60877600
H	5.62686900	0.93816000	0.40012000
H	6.43045500	-0.53331200	0.98669600
S	-1.81782800	0.53819700	-1.13801900
Si	-2.78127200	-1.05195500	0.00151500
C	-2.10717800	-0.96953500	1.78104200
C	-4.65251300	-0.69681200	-0.04430900
C	-2.36010800	-2.73452100	-0.77781700
C	-2.59933200	-2.12972300	2.64812100
C	-2.40426000	0.36369600	2.46628600
H	-1.01220900	-1.06916000	1.67796600
C	-5.47701600	-1.94535600	0.28011100
C	-5.14297200	-0.05945600	-1.34438700
H	-4.80787100	0.03720100	0.76522200
C	-0.86472000	-3.03816900	-0.70874200
C	-2.85036800	-2.84318300	-2.22128700
H	-2.89632300	-3.48580800	-0.17194600
H	-2.39689200	-3.11232100	2.20318100
H	-2.11629100	-2.10906000	3.63511600
H	-3.68199700	-2.05939400	2.82374000
H	-2.07943500	1.22893700	1.87364500
H	-3.48176400	0.47889300	2.64978000
H	-1.90588800	0.41947300	3.44479800
H	-5.17369600	-2.43010800	1.21665600
H	-6.54244000	-1.69207200	0.37200600
H	-5.39436200	-2.69553600	-0.51849800
H	-4.63990300	0.89185400	-1.55391100
H	-4.97564600	-0.71841200	-2.20748600
H	-6.22303500	0.13855900	-1.29328300
H	-0.47228700	-3.03155800	0.31825300
H	-0.64290900	-4.02643800	-1.13646000
H	-0.29457100	-2.29876200	-1.29173000
H	-3.93993200	-2.74522000	-2.30473300
H	-2.39741000	-2.06318400	-2.84959300
H	-2.57449900	-3.81434500	-2.65600900

TS II₂-P₂(RSH)



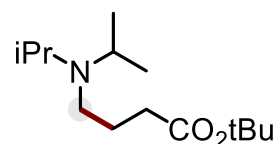
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$$G_{\text{Corr.}} = 0.616775$$

C	4.92057300	-0.91682800	-1.05108100
H	4.34834200	-0.64760300	-1.95862700
N	4.10024800	-1.29549000	0.08319500
C	3.61967900	-2.68842400	0.03245800
C	4.67928800	-3.62367300	0.60303600
C	3.16172700	-3.17156400	-1.34550900
H	2.74719600	-2.74939400	0.69507600
H	4.92827800	-3.34091700	1.63212700
H	4.32767300	-4.66296100	0.59870300
H	5.60176600	-3.58374900	0.00862700
H	2.43501600	-2.49376400	-1.80832900
H	4.00436000	-3.28742900	-2.03831600
H	2.68447600	-4.15421400	-1.24661800
C	3.18144900	-0.28168700	0.61388200
C	1.89144400	-0.20176600	-0.27494400
H	2.18436300	-0.02211300	-1.31878200
H	1.40877500	-1.18749700	-0.22250500
C	0.91179800	0.83283700	0.13730000
H	0.51592800	0.79812800	1.15538800
C	0.97563600	2.18882700	-0.44365500

O	1.52157800	2.45434900	-1.49921600
O	0.29728800	3.05095800	0.32478200
C	0.02140600	4.42599600	-0.10747700
C	1.32159800	5.19489500	-0.26784100
C	-0.81058900	4.39766300	-1.37780400
C	-0.78891500	4.98066800	1.05032300
H	1.92757800	5.10859500	0.64257000
H	1.90467600	4.83274100	-1.11805000
H	1.09398600	6.25615000	-0.42492900
H	-1.70208600	3.77450000	-1.23183600
H	-1.13909500	5.41647400	-1.61605100
H	-0.24315000	4.00834800	-2.22747000
H	-1.07022100	6.01975400	0.84515300
H	-1.70388300	4.39448400	1.19692000
H	-0.20541100	4.95458800	1.97788300
H	-0.29365800	0.41267700	-0.57438400
S	-1.49976300	0.08177600	-1.45499200
Si	-2.59402000	-1.05930000	0.04757200
C	-2.07874100	-0.40530200	1.76109500
C	-4.44603200	-0.75215700	-0.27831100
C	-2.13984700	-2.89968300	-0.10390600
C	-2.73689000	-1.18011900	2.90418100
C	-2.32818000	1.09360100	1.92396400
H	-0.99068400	-0.58581700	1.82155200
C	-5.32498700	-1.83516500	0.35330100
C	-4.80557500	-0.57173100	-1.75328900
H	-4.65568400	0.20238600	0.23518700
C	-0.65521600	-3.14340000	0.16100000
C	-2.53028900	-3.48785900	-1.45931600
H	-2.72280500	-3.41456900	0.67976200
H	-2.57506900	-2.26366200	2.83544600
H	-2.34171200	-0.84920700	3.87482600
H	-3.82162600	-1.00464400	2.92684500
H	-1.88021300	1.68932200	1.11803600
H	-3.40542300	1.31192800	1.93711800
H	-1.91502200	1.45866300	2.87580000
H	-5.11757000	-1.99122900	1.41925800
H	-6.38800700	-1.57215900	0.26080300
H	-5.18994400	-2.80176300	-0.15129200
H	-4.26034500	0.26062800	-2.21373100
H	-4.58372600	-1.47543500	-2.33764900
H	-5.88014900	-0.36962000	-1.86631500
H	-0.32012700	-2.74545700	1.12913400
H	-0.42160700	-4.21760600	0.14700100
H	-0.04781700	-2.67208800	-0.62627500
H	-3.61043300	-3.44030700	-1.64500000
H	-2.02840500	-2.95242100	-2.27781600
H	-2.23216400	-4.54367600	-1.52842800
H	5.57761300	-1.75217900	-1.31490200
H	5.57321100	-0.07551700	-0.80208300
C	3.87313300	1.08005900	0.64601300
H	4.05275700	1.48794800	-0.35432800
H	3.24772800	1.80273200	1.18496300
H	4.82972000	1.00527900	1.17807600
C	2.80111600	-0.63958400	2.05406300
H	2.16139400	-1.52709400	2.12564000
H	3.71117600	-0.82461300	2.63754400
H	2.25833300	0.18750200	2.52634400

P₁



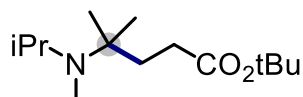
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$$G_{\text{Corr.}} = 0.363292$$

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C	3.58062900	-1.06806100	0.20384300
H	3.02840400	-2.02122400	0.18571800
H	3.37768700	-0.83661300	2.36789000

H	4.78930100	-1.78189900	1.86053800
H	4.80164200	-0.02227100	1.67991000
C	4.68662000	-1.18120600	-0.83747900
H	4.25996900	-1.34477700	-1.83383600
H	5.30131300	-0.27216600	-0.87655100
H	5.35805200	-2.01581300	-0.60073000
N	2.59804100	-0.05132200	-0.17198700
C	3.00938500	1.35287900	-0.11383600
C	2.69089500	2.08252700	1.19475900
C	2.42487400	2.11073600	-1.30044600
H	4.10341200	1.35382300	-0.22980900
H	3.05025200	1.53303400	2.07157200
H	3.16429000	3.07232900	1.19777200
H	1.61158300	2.24310200	1.31446000
H	2.75045000	1.65592500	-2.24325500
H	1.32618000	2.08442400	-1.27661600
H	2.73218200	3.16424600	-1.29106700
C	1.23687500	-0.34774800	0.23051300
H	1.19761800	-0.81459600	1.23760900
H	0.67075800	0.58805700	0.31410900
C	0.51990300	-1.24524200	-0.77221700
H	0.49565200	-0.72947800	-1.74195600
H	1.09790400	-2.16812700	-0.92034100
C	-1.86580700	-0.46469400	-0.39534800
O	-1.64733100	0.60767500	-0.92047300
O	-3.01715500	-0.80918700	0.19400200
C	-4.17210100	0.09732200	0.24203900
C	-3.82420400	1.34373100	1.03740800
C	-4.64415300	0.41656200	-1.16606400
C	-5.21355900	-0.72755900	0.97681200
H	-3.42664600	1.06875600	2.02165200
H	-3.09169200	1.96615800	0.51789000
H	-4.73499000	1.93451800	1.19295900
H	-4.82350600	-0.50880400	-1.72644100
H	-5.59111200	0.96683100	-1.10948900
H	-3.91944900	1.02789100	-1.70948200
H	-6.14043900	-0.15179400	1.07913800
H	-5.43553100	-1.64919800	0.42694300
H	-4.85846200	-0.99580700	1.97832500
C	-0.88837400	-1.61224000	-0.33837000
H	-1.30497100	-2.40582800	-0.97385500
H	-0.90162500	-2.02204500	0.68149800

P₂



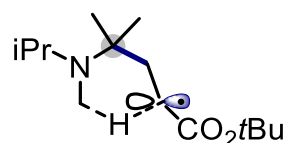
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G_{Corr.} = 0.363508

C	4.88302500	0.38055000	0.68295400
C	3.75984200	-0.52063300	0.16372000
H	3.31958300	-1.00630000	1.04326300
H	4.50259400	1.21475500	1.28294700
H	5.56163200	-0.20559300	1.31456600
H	5.48368700	0.79814000	-0.13490100
C	4.32834200	-1.62741300	-0.71667500
H	3.54204400	-2.33905400	-0.99319100
H	4.75103000	-1.21613800	-1.64320900
H	5.13015100	-2.17074900	-0.20027000
N	2.66460400	0.16889700	-0.54273000
C	3.13005400	1.23079400	-1.41204200
H	4.03626100	0.89907200	-1.93073000
C	1.43058500	0.43502500	0.23754000
C	0.80934400	-0.93575000	0.58888000
H	0.77163400	-1.53407900	-0.33162000
H	1.47392100	-1.46748900	1.28042600
C	-1.70550500	-0.82089900	0.21627300
O	-1.70782500	-1.39285500	-0.85410400
O	-2.70531300	-0.06229100	0.68216200
C	-3.92696200	0.17544700	-0.09958800
C	-3.57941300	0.92244700	-1.37578100

C	-4.64875300	-1.13458400	-0.36441400
C	-4.74879900	1.05617100	0.82429800
H	-3.02235400	1.83797300	-1.14093400
H	-2.98493400	0.30845300	-2.05729700
H	-4.50594200	1.21184200	-1.88622700
H	-4.80861900	-1.67713400	0.57509200
H	-5.63120700	-0.91815900	-0.80117200
H	-4.09352600	-1.77371200	-1.05498100
H	-5.69816900	1.31689000	0.34285200
H	-4.96695600	0.53486400	1.76331800
H	-4.21052800	1.98226800	1.05602200
C	-0.58135600	-0.91148100	1.21865300
H	-0.74768400	-1.85891200	1.75066400
H	-0.69392000	-0.12112000	1.96941700
C	1.70685700	1.25200700	1.50772700
H	2.33532700	0.70159100	2.21893700
H	2.21408600	2.19287600	1.25735700
H	0.77645800	1.51730300	2.02524900
C	0.44337500	1.21867500	-0.62695700
H	0.23076000	0.69555900	-1.56779500
H	-0.50157200	1.35567300	-0.08725200
H	0.81159500	2.22451200	-0.85648000
H	3.37758900	2.17899800	-0.89500100
H	2.39613400	1.45441800	-2.19193200

TS II₂-H_{[1-5]p}



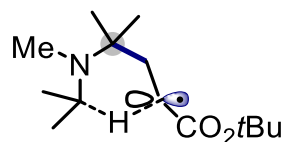
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G_{Corr.} = 0.348372

N	2.40868300	0.22549900	0.54861500
C	2.63406300	1.43069600	-0.27350400
C	3.39853600	2.46934000	0.53805800
C	1.36933400	2.03202300	-0.88347100
H	3.29055700	1.12541000	-1.09448100
H	4.31951600	2.04154600	0.94933200
H	3.66311400	3.32270300	-0.09718800
H	2.79894000	2.85514100	1.37234900
H	0.82186600	1.31756100	-1.50703900
H	0.67771800	2.39004100	-0.10855500
H	1.63676000	2.89478800	-1.50518300
C	2.41520000	-1.12274000	-0.06609600
C	1.03562900	-1.42970800	-0.72096000
H	0.93003900	-0.82142300	-1.62858500
H	1.07220600	-2.48150000	-1.04922700
C	-0.14982200	-1.18687800	0.16763700
H	-0.40793900	-1.97572900	0.87872800
C	-1.31855000	-0.53285400	-0.41597800
O	-1.34220000	0.05234100	-1.49125500
O	-2.37354300	-0.59629600	0.42956800
C	-3.60990900	0.13357100	0.16720300
C	-3.33081400	1.62657000	0.08522200
C	-4.28959100	-0.39963800	-1.08368200
C	-4.45175600	-0.17600500	1.39361900
H	-2.76917100	1.95422000	0.96939700
H	-2.76137300	1.88378300	-0.81164700
H	-4.28202100	2.17255100	0.06543900
H	-4.42124700	-1.48585500	-1.00864300
H	-5.28262900	0.05705000	-1.17801300
H	-3.71305100	-0.17318200	-1.98360200
H	-5.42629100	0.31957200	1.31474800
H	-4.61698400	-1.25577000	1.48481400
H	-3.95357400	0.17773500	2.30369100
C	1.46833800	0.36027500	1.58231600
H	1.64683400	-0.26026700	2.46454200
H	1.21885500	1.38934300	1.84253400
H	0.36814900	-0.26023200	1.02722500
C	2.71451600	-2.16128000	1.01958100

H	1.92600100	-2.24034300	1.77420800
H	2.81720800	-3.15010700	0.55790900
H	3.65511700	-1.91843600	1.52911900
C	3.50092300	-1.24580000	-1.12823100
H	4.47734900	-0.94539900	-0.72690700
H	3.57304800	-2.29189200	-1.44672900
H	3.28957000	-0.65358300	-2.02532100

TS II₂-H_{[1-5]t}

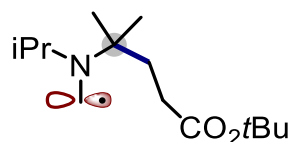


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G_{Corr.} = 0.349522

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C	-2.62741600	-0.78735300	-0.25786800
C	-1.28465900	-1.55667000	-0.13221500
H	-1.08584700	-1.75982200	0.92868900
H	-1.41875800	-2.53191500	-0.62622500
C	-0.11715900	-0.81416800	-0.71662700
H	0.05692900	-0.91503000	-1.79011400
C	1.10904100	-0.73124800	0.07509000
O	1.18145900	-0.92984800	1.28146700
O	2.15079100	-0.32964300	-0.68823300
C	3.46370400	-0.05012100	-0.11245600
C	3.36820300	1.09702800	0.88067300
C	4.05232100	-1.30709000	0.50811200
C	4.28085600	0.36910200	-1.32262400
H	2.89448000	1.96731000	0.40900800
H	2.79462500	0.81683300	1.76814100
H	4.37784400	1.38943400	1.19433000
H	4.04357800	-2.12771600	-0.21945300
H	5.09482800	-1.11536800	0.79067400
H	3.49891000	-1.61587300	1.39812400
H	5.30494800	0.61289200	-1.01721000
H	4.32112900	-0.44091900	-2.05994800
H	3.84003000	1.25217500	-1.79950600
C	-1.47613900	1.38809900	-0.13030900
H	-0.62126500	0.44540100	-0.61900000
C	-2.98700300	-0.63450800	-1.73594500
H	-2.20914900	-0.13930200	-2.32412300
H	-3.13268800	-1.63100100	-2.17054000
H	-3.92160900	-0.07171100	-1.85081700
C	-3.73352100	-1.61361800	0.38987100
H	-4.67974300	-1.05789600	0.40280600
H	-3.88734700	-2.52694900	-0.19599000
H	-3.49187000	-1.92290300	1.41216000
C	-1.89450100	2.30831300	-1.25707100
H	-2.34953500	3.21703900	-0.83075400
H	-1.02389200	2.62516000	-1.84559600
H	-2.62886500	1.86668700	-1.93208200
C	-0.56062100	2.09389000	0.84078400
H	0.27227700	2.53351600	0.27629400
H	-1.06238900	2.92340000	1.36257700
H	-0.13392100	1.41735300	1.58994800
C	-2.60050600	0.49925000	1.86336000
H	-1.82724100	-0.12268300	2.34850200
H	-2.51996600	1.51178900	2.26410000
H	-3.58117500	0.12135900	2.16329800

H_{[1-5]p}

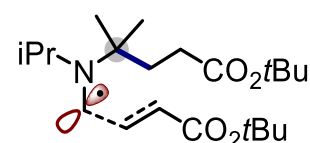


E = -755.2215814

G_{Corr.} = 0.350148

N	3.17494100	-0.24531600	0.33065600
C	3.51943500	0.96516600	-0.43357700
C	4.94209200	0.86520200	-0.97116900
C	3.31236200	2.26510800	0.34083600
H	2.84197200	0.99807900	-1.29447500
H	5.06045800	-0.02368900	-1.60142100
H	5.19407500	1.75132100	-1.56639600
H	5.66493200	0.79627300	-0.14823100
H	2.31329200	2.31342500	0.78766400
H	4.04864300	2.38371100	1.14434500
H	3.42758300	3.11784600	-0.33874100
C	1.97113500	-1.01511500	-0.07408600
C	0.72680500	-0.13854700	0.16646400
H	0.75253900	0.19371000	1.21501100
H	0.80113400	0.77134100	-0.44516400
C	-0.61056800	-0.79927500	-0.11885500
H	-0.66937700	-1.18286900	-1.14743200
C	-1.77754500	0.13683000	0.06742000
O	-1.68656200	1.30686200	0.37445500
O	-2.92656200	-0.51150100	-0.15810400
C	-4.23154200	0.15553100	-0.05124800
C	-4.45387400	0.63819500	1.37173700
C	-4.32878600	1.27797500	-1.07014700
C	-5.20495000	-0.95806500	-0.39308700
H	-4.31225900	-0.18679300	2.08008600
H	-3.77653700	1.45442900	1.63489700
H	-5.48566500	0.99635000	1.47094500
H	-4.09939100	0.90155100	-2.07423900
H	-5.35520400	1.66407000	-1.07973000
H	-3.65025200	2.10146000	-0.83395200
H	-6.23297800	-0.58111700	-0.34701700
H	-5.01893000	-1.33792300	-1.40414200
H	-5.10710300	-1.78858900	0.31522300
C	3.64999100	-0.31430400	1.62832200
H	3.59427300	-1.26120800	2.15225100
H	4.47902000	0.34120900	1.87592500
H	-0.78783100	-1.66896300	0.52812200
C	1.88092200	-2.30116700	0.74441900
H	1.63488300	-2.10997600	1.79528700
H	1.09890200	-2.94735800	0.33199000
H	2.82478000	-2.85727900	0.69756500
C	2.10692900	-1.42138000	-1.54519100
H	3.04900100	-1.96267800	-1.69558100
H	1.28888700	-2.09007600	-1.83621400
H	2.08710900	-0.56885700	-2.23301300

TS H_{[1-5]p}-bisAc



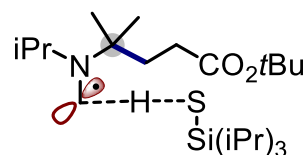
E = -1179.497962

G_{Corr.} = 0.51575

N	-0.57295600	1.71454800	0.34724200
C	-0.84655500	1.92700100	-1.08764300
C	-1.92455000	2.98702300	-1.27726900
C	-1.19555200	0.63771000	-1.82387000
H	0.07884100	2.31601500	-1.52666600
H	-1.64420100	3.92469300	-0.78374800
H	-2.07725700	3.18689900	-2.34429800
H	-2.88548300	2.65830000	-0.86054300
H	-0.39682600	-0.10742200	-1.73443100
H	-2.12209800	0.19470100	-1.43863900
H	-1.34681800	0.84928900	-2.88936600
C	0.82171500	1.86998200	0.84062900
C	1.68885500	0.79331400	0.16084800

H	1.22909200	-0.18611400	0.36002200	H	0.06717800	1.40955900	-2.11157500
H	1.65189100	0.93044700	-0.92822900	H	-1.40064800	2.40211600	-2.04240200
C	3.14699000	0.75760400	0.58457200	H	-0.08257100	2.86064500	-3.12911600
H	3.64055200	1.72925400	0.44102600	C	1.44339400	2.28246700	0.99513900
C	3.94886200	-0.26141900	-0.18584500	C	2.12268900	1.18214700	0.15443400
O	3.51185600	-0.94880300	-1.08479800	H	1.38341200	0.39089600	-0.03828600
O	5.20686300	-0.29153800	0.26587300	H	2.39829000	1.58764000	-0.82789600
C	6.21909900	-1.19427200	-0.30271000	C	3.36253800	0.55940100	0.77410100
C	5.80486300	-2.63954500	-0.08792300	H	4.09287200	1.31962200	1.08793400
C	6.44827700	-0.86377200	-1.76729400	C	4.08683400	-0.36082300	-0.17653200
C	7.45471400	-0.86722800	0.51602900	O	3.83125600	-0.47957500	-1.35608800
H	5.58688300	-2.82000500	0.97145900	O	5.06070100	-1.01166100	0.46962100
H	4.92749300	-2.90428500	-0.68317400	C	5.95144900	-1.95945400	-0.21494900
H	6.63369400	-3.29575000	-0.37938900	C	5.14792200	-3.12723300	-0.76041000
H	6.67698500	0.20207000	-1.88618900	C	6.74575000	-1.24267900	-1.29318300
H	7.30898100	-1.43712300	-2.13204000	C	6.86907800	-2.42118500	0.90272900
H	5.57987300	-1.11365900	-2.38177800	H	4.53879400	-3.57450600	0.03402100
H	8.29563300	-1.48637600	0.18377900	H	4.49439400	-2.82343400	-1.58179200
H	7.73056000	0.18666600	0.39650500	H	5.83882200	-3.89432100	-1.13043000
H	7.27760600	-1.06343300	1.57956700	H	7.25897000	-0.37001000	-0.87166000
H	3.26400400	0.52304500	1.65080500	H	7.50778100	-1.92508100	-1.68852800
C	0.86442800	1.70467600	2.35669100	H	6.10884100	-0.91793000	-2.11973300
H	0.62632800	0.68207200	2.67331600	H	7.59382900	-3.14547400	0.51399500
H	1.86972200	1.94007300	2.72035200	H	7.41851400	-1.57343900	1.32772900
H	0.17247600	2.39811400	2.84865600	H	6.29344600	-2.90045500	1.70268900
C	1.30560000	3.28691900	0.51596900	C	-1.04145500	2.29857900	0.68606100
H	0.60727400	4.02227000	0.93339600	H	-1.21553700	2.20294100	1.75589200
H	2.28870000	3.47053300	0.96378500	H	-1.86856700	2.74943900	0.13704300
H	1.39884800	3.47311300	-0.55966900	H	3.12939500	-0.01746900	1.67794000
C	-1.53308300	1.07519300	1.07812000	C	1.09374400	1.74753700	2.38038400
H	-1.47203600	1.10084200	2.15932800	H	0.49628700	0.82804700	2.33384100
H	-2.53393500	1.05942300	0.65370500	H	2.01646100	1.52006900	2.92368200
C	-1.70612200	-1.39436400	1.15557900	H	0.55141300	2.49639000	2.96960000
H	-0.75210400	-1.53590400	1.65816900	C	2.34883500	3.50469300	1.17500200
H	-1.67863600	-1.30903800	0.07410800	H	1.80880900	4.29074600	1.71651400
C	-2.87251900	-1.61332600	1.82043900	H	3.23703600	3.24701900	1.76266500
H	-2.88285700	-1.83459100	2.88564200	H	2.69610800	3.91958800	0.22190700
C	-4.19678200	-1.48668800	1.23250000	Si	-3.36877100	-0.97736400	-0.02070200
O	-5.23462900	-1.71240800	1.84194600	S	-1.21691100	-0.76708600	0.08422700
O	-4.15877800	-1.07074700	-0.05669000	H	-1.21808700	0.71058700	0.33219900
C	-5.38205500	-0.81322700	-0.81081800	C	-4.04095500	0.47272100	-1.06812200
C	-6.18326700	-2.09441400	-0.97785400	C	-5.53206000	0.75246600	-0.87738000
C	-6.18466200	0.29511800	-0.14735300	C	-3.71429700	0.30209800	-2.55102700
C	-4.86477500	-0.34136400	-2.15970600	H	-3.48598500	1.35456000	-0.70289300
H	-5.55630800	-2.87741600	-1.42135400	H	-5.79316300	0.96469400	0.16673600
H	-6.57475700	-2.45138500	-0.02238100	H	-5.84386700	1.62010200	-1.47665100
H	-7.02556100	-1.90834300	-1.65568600	H	-6.14866600	-0.09647000	-1.20409400
H	-5.54283900	1.16781100	0.03229500	H	-2.65292000	0.07632400	-2.71975500
H	-6.99736100	0.60386200	-0.81639200	H	-4.30253300	-0.51468900	-2.99338600
H	-6.61579300	-0.02872700	0.80282800	H	-3.95697800	1.21392600	-3.11585700
H	-5.70567600	-0.15687100	-2.83824900	C	-3.69572900	-2.64289500	-0.88376600
H	-4.29578600	0.59166200	-2.05523400	C	-5.17405300	-3.03216700	-0.82434600
H	-4.21179100	-1.09810000	-2.61116600	C	-2.81465800	-3.79504800	-0.40244400

TS H_{[1-5]p}-P₂(RSH)

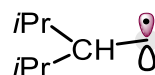


E = -1799.001666

G_{Corr.} = 0.614254

N	0.20793200	2.71299200	0.28602000
C	0.32732000	3.30335700	-1.05956900
C	-0.23189600	4.72077200	-1.07496500
C	-0.30799900	2.43864100	-2.14300300
H	1.39928400	3.36648000	-1.27819300
H	0.26921800	5.35090800	-0.33150700
H	-0.09364900	5.17309800	-2.06397200
H	-1.30697000	4.72344700	-0.85522100

α -C I₁

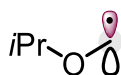


E = -314.8686079

G_{Corr.} = 0.191976

C	-1.82762000	-1.02602400	-0.67600300
C	-1.46339400	0.07139800	0.31696000
H	-2.01514400	-0.13563500	1.25030800
H	-1.45863300	-2.00830000	-0.35267600
H	-2.91680600	-1.09480400	-0.78875300
H	-1.41281600	-0.81739600	-1.67156700
C	-1.93896700	1.42723700	-0.19130400
H	-1.69825400	2.23181000	0.51552700
H	-1.48251300	1.68194700	-1.15731900
H	-3.02573900	1.42542500	-0.34101500
C	1.04010900	0.33812600	-0.41330500
C	1.48465900	-0.92475900	-1.14923400
C	2.26730200	1.07739100	0.11198900
H	0.54842500	0.99916300	-1.14518900
H	0.64408300	-1.53642500	-1.49265000
H	2.08760600	-0.65881000	-2.02674100
H	2.10970200	-1.55749600	-0.50528400
H	1.99908900	2.04934100	0.54452300
H	2.77287700	0.49263100	0.89386800
H	2.99736700	1.25291200	-0.68815000
C	0.36840900	-1.10515900	1.54974300
H	-0.39859200	-1.60334800	2.14122300
H	1.40195400	-1.38120700	1.74911400
C	0.02571900	0.08855800	0.73162800
H	0.11009200	0.97958200	1.39193000

α -O I₁

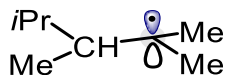


E = -232.908669

G_{Corr.} = 0.091096

C	0.60416500	1.43032800	-0.13316000
C	0.37709100	0.00383000	0.32353100
H	0.17169600	-0.01477200	1.40859900
H	-0.27164900	2.05589900	0.07215600
H	1.46792500	1.86382500	0.38326000
H	0.79900000	1.45125800	-1.21268500
C	1.54186200	-0.90195000	0.00289900
H	1.34714300	-1.92694500	0.33392900
H	1.72054800	-0.91431100	-1.07928700
H	2.45059200	-0.54179300	0.49703300
C	-1.96781200	-0.08492100	0.07927800
H	-2.04448100	0.28309900	1.10356200
H	-2.81695200	-0.53125800	-0.42577200
O	-0.76945700	-0.55109100	-0.33951100

α -C I₂



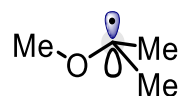
E = -314.8826651

G_{Corr.} = 0.192038

C	-1.11029600	-0.59827500	-0.03423300
C	-2.53698900	-0.27038600	-0.45766300
C	-1.00668000	-0.71048300	1.48196200
H	-0.86156000	-1.58679700	-0.45518100
H	-2.61023700	-0.11065000	-1.54167700
H	-3.21935300	-1.08714200	-0.19134300
H	-2.90567000	0.63611300	0.04090700
H	-0.01592500	-1.06165300	1.79756000
H	-1.19148500	0.25605100	1.97115300

H	-1.75001900	-1.41805400	1.87020400
C	1.32916100	-0.00817500	-0.28121700
C	-0.39533100	1.85137000	-0.31436600
H	0.38212900	2.51506600	-0.71145400
H	-1.34667200	2.15490400	-0.76490600
H	-0.46804700	2.03828400	0.76491900
C	2.13455500	0.64277500	0.78984200
H	1.75210200	1.62516500	1.08561000
H	2.17499000	0.02317900	1.70575500
H	3.18206200	0.77133800	0.47581300
C	1.84228200	-1.30613600	-0.80237900
H	1.34963600	-1.60087500	-1.73850300
H	2.92615600	-1.26658500	-0.98422200
H	1.68567800	-2.13372200	-0.08385600
C	-0.07517800	0.39425300	-0.63360800
H	-0.17292900	0.27572400	-1.73080900

α -O I₂

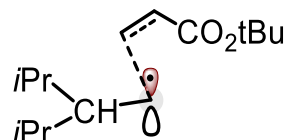


E = -232.912363

G_{Corr.} = 0.090838

C	-0.46253900	0.00902200	0.20110500
C	1.90398200	-0.18234000	0.05741600
H	2.01744100	0.14488900	1.10082800
H	2.63617800	-0.96453600	-0.15438600
H	2.09354700	0.66985800	-0.60897200
C	-0.42802000	1.47753300	-0.04166100
H	0.40360900	1.98489300	0.46208600
H	-0.34503200	1.71365200	-1.12009200
H	-1.35718000	1.93056700	0.31870600
C	-1.72636300	-0.74623800	0.01627500
H	-1.64012000	-1.76146000	0.41974000
H	-2.55979000	-0.24119900	0.51643300
H	-1.99509400	-0.84274500	-1.05220000
O	0.62801000	-0.74772300	-0.16011900

α -C TS I₁-II₁



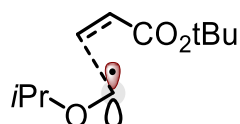
E = -739.1428412

G_{Corr.} = 0.358198

C	-3.72050500	-0.55775500	1.57727800
C	-2.22555100	-0.61730900	1.28411000
H	-1.93406900	-1.68202000	1.26259800
H	-4.32445700	-0.99547100	0.77195300
H	-3.94801000	-1.10872300	2.49815900
H	-4.05660100	0.47710800	1.72879000
C	-1.43353400	0.03247600	2.41245100
H	-0.35540400	-0.10989300	2.26528300
H	-1.63116400	1.11185200	2.47780100
H	-1.70328200	-0.40496500	3.38169400
C	-2.24404300	1.40593500	-0.39264200
C	-3.64010800	1.55045600	-0.99482800
C	-1.22094100	2.07371300	-1.30758700
H	-2.23079600	1.94673900	0.56803300
H	-4.41314000	1.04949700	-0.40330900
H	-3.91229000	2.61069800	-1.07116800
H	-3.67748500	1.13278500	-2.01017700
H	-0.22188800	2.09556100	-0.85115800
H	-1.13259400	1.53314700	-2.26164900

H	-1.50961700	3.10594300	-1.54214000
C	-2.16535000	-0.99324500	-1.19951700
H	-2.88255900	-1.79607900	-1.01999000
H	-2.11913800	-0.64235200	-2.22996500
C	-0.33268200	-2.41049800	-1.49448100
H	-0.53261500	-2.89125000	-0.53846400
H	-0.82529100	-2.82058900	-2.37110900
C	0.72866000	-1.57153900	-1.61617300
H	1.00077100	-1.12723700	-2.57153800
C	1.46851600	-1.12181300	-0.43377300
O	1.34284000	-1.58418700	0.68944700
O	2.29848100	-0.11327700	-0.75782000
C	3.13109800	0.55946900	0.23994200
C	2.27366300	1.15206800	1.34737200
C	4.17463500	-0.40683800	0.77362900
C	3.78605900	1.66710500	-0.56649800
H	1.43890200	1.72576500	0.92232500
H	1.87046600	0.38082600	2.00808800
H	2.88586900	1.83933700	1.94380000
H	4.75896000	-0.83006400	-0.05195700
H	4.86207900	0.13264300	1.43655100
H	3.71386300	-1.22114400	1.33932800
H	4.46957700	2.24046100	0.06998200
H	4.35683300	1.24927500	-1.40351400
H	3.02770400	2.35005700	-0.96810100
C	-1.81275800	-0.05644000	-0.09280900
H	-0.70814000	-0.00691400	-0.05201000

α -O TS I₁-II₁

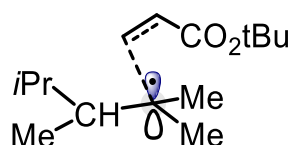


$$E = -657.1845584$$

$$G_{\text{Corr.}} = 0.255107$$

C	-2.67060400	-2.04283500	-0.99068400
C	-1.95499300	-1.08987600	-0.05701700
H	-1.17917600	-0.53700300	-0.61196200
H	-3.15446700	-1.50687200	-1.81496500
H	-1.95635000	-2.75455100	-1.42122300
H	-3.43683400	-2.60622500	-0.44413200
C	-1.35024700	-1.78394900	1.13998100
H	-0.78823100	-1.07922700	1.76290700
H	-2.14143300	-2.24185800	1.74618900
H	-0.66818800	-2.57857900	0.81485100
C	-3.10114100	0.96376200	-0.30479900
H	-2.81194400	0.91620300	-1.35627800
H	-3.97024500	1.54711300	-0.01435100
C	-1.40567300	2.56470100	0.32403100
H	-1.38431600	2.86955900	-0.71960300
H	-2.11771300	3.06138200	0.97610200
C	-0.38876200	1.82753600	0.83714000
H	-0.33268400	1.58529800	1.89597100
C	0.60206200	1.21801100	-0.04790500
O	0.65138200	1.37817900	-1.25878000
O	1.43315900	0.41661100	0.64665800
C	2.48072100	-0.36600000	-0.00854300
C	1.87711500	-1.33141700	-1.01765900
C	3.50579800	0.56185400	-0.63901100
C	3.09731100	-1.13399600	1.14758100
H	1.10276700	-1.94887100	-0.54261800
H	1.44103400	-0.80773200	-1.87213000
H	2.66344100	-2.00331800	-1.38277200
H	3.88006300	1.27409400	0.10593800
H	4.35546400	-0.03007100	-1.00061200
H	3.08338300	1.11647100	-1.48072900
H	3.91463700	-1.76706100	0.78361500
H	3.49852800	-0.44431200	1.89884800
H	2.34811600	-1.77472200	1.62837100
O	-2.89646300	-0.12184900	0.45585700

α -C TS I₂-II₂

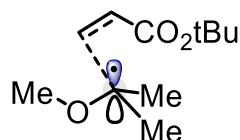


$$E = -739.1518953$$

$$G_{\text{Corr.}} = 0.358605$$

C	3.72925800	-0.93368400	0.41912200
C	5.25488400	-0.97962500	0.44942900
C	3.21035700	-1.88458600	-0.65532400
H	3.38493700	-1.31321800	1.39362500
H	5.66868000	-0.26792600	1.17567300
H	5.60325200	-1.98211500	0.72598300
H	5.68694400	-0.74727800	-0.53283900
H	2.11606200	-1.94784900	-0.67317600
H	3.54706000	-1.58300400	-1.65661400
H	3.59580200	-2.89676000	-0.48074600
C	1.72797800	0.70653600	0.56614400
C	0.57686800	0.32101600	-1.41532200
H	0.48683200	1.39919900	-1.52697500
H	1.43377100	-0.15378500	-1.88317000
C	-0.53115300	-0.41963700	-1.12353700
H	-0.51460100	-1.50767600	-1.15427400
C	-1.75621800	0.21381400	-0.64340200
O	-1.90521800	1.41630700	-0.48100300
O	-2.70112600	-0.71227200	-0.38675000
C	-4.00424700	-0.35199200	0.17081300
C	-3.82508200	0.27914000	1.54216000
C	-4.76333800	0.54819000	-0.79007200
C	-4.70054700	-1.69609000	0.29517600
H	-3.22014400	-0.37427500	2.18316200
H	-3.34497000	1.25887300	1.47755500
H	-4.80753700	0.40208100	2.01403200
H	-4.81202000	0.08656300	-1.78359300
H	-5.78970300	0.67743900	-0.42525600
H	-4.29688500	1.53223200	-0.87773100
H	-5.70491900	-1.55978600	0.71218400
H	-4.79337900	-2.17466400	-0.68646800
H	-4.13653700	-2.36392800	0.95638200
C	3.71660800	1.21558400	-0.96254000
H	3.31292400	2.22820300	-1.06005100
H	4.80774200	1.30827400	-0.94909500
H	3.44609500	0.66772900	-1.87297100
C	1.29474700	2.12782700	0.78040700
H	1.69303600	2.82560900	0.03595600
H	0.20192500	2.21615600	0.77477300
H	1.65154100	2.47025500	1.76843000
C	1.06838400	-0.23893900	1.52207400
H	1.52387400	-0.13253200	2.52244700
H	0.00167400	-0.00507200	1.62991400
H	1.15502600	-1.29230200	1.23508300
C	3.21281400	0.51648200	0.30228900
H	3.68640400	1.05306500	1.15528300

α -O TS I₂-II₂



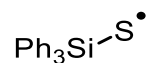
$$E = -657.191497$$

$$G_{\text{Corr.}} = 0.255301$$

C	-2.87608000	0.17799800	0.42237900
C	-1.49402700	1.16514300	-1.29426000
H	-1.67718400	0.23320500	-1.82437900

H	-2.22549400	1.95808200	-1.42305900
C	-0.26197400	1.43136300	-0.78804600
H	-0.01577000	2.39762900	-0.35309000
C	0.74434200	0.37914700	-0.69493000
O	0.60401700	-0.76463700	-1.10887000
O	1.85027000	0.82725700	-0.06666500
C	2.97029200	-0.05792600	0.24638000
C	2.50802100	-1.17082600	1.17376200
C	3.60296500	-0.58730800	-1.03006100
C	3.93647400	0.86332800	0.97094700
H	1.99358500	-0.74639900	2.04524300
H	1.83480100	-1.86731000	0.66710600
H	3.38148200	-1.72828100	1.53332500
H	3.86783900	0.24409600	-1.69425800
H	4.52399500	-1.12708300	-0.77779600
H	2.93285400	-1.26700500	-1.56176900
H	4.83576800	0.30846900	1.26197300
H	4.23532400	1.69515900	0.32292300
C	3.47346100	1.27518300	1.87504800
C	-2.53407000	-2.07005200	-0.29802100
H	-1.55530300	-1.81164900	-0.72548600
H	-2.39080800	-2.53756900	0.68432700
H	-3.04990500	-2.77301900	-0.95452600
C	-1.89828600	0.00519300	1.53174300
H	-1.01494700	-0.57678500	1.24249900
H	-1.55265200	0.98826200	1.86834900
H	-2.36771900	-0.50046100	2.39263000
C	-3.91656300	1.23360500	0.54429100
H	-4.64845700	0.97362400	1.32727500
H	-3.46507700	2.19425400	0.81563400
H	-4.46710300	1.35121000	-0.39605900
O	-3.37119400	-0.92532000	-0.20334100

Ph₃Si·



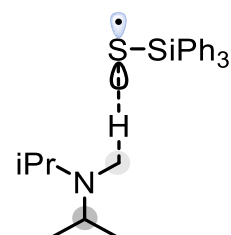
$$E = -1382.281865$$

$$G_{\text{Corr.}} = 0.222907$$

Si	0.00385900	-0.00721600	0.62072100
S	0.15155100	0.34503300	2.73199200
C	-1.73835900	-0.43953200	0.08444200
C	-2.66316400	-1.02304600	0.95910000
C	-2.13097700	-0.21613100	-1.24402400
C	-3.93791900	-1.37787100	0.52290300
H	-2.38905800	-1.19460200	2.00039400
C	-3.40369000	-0.56787500	-1.68549000
H	-1.43383600	0.24504100	-1.94584300
C	-4.30852100	-1.15120900	-0.80056300
H	-4.64371000	-1.82771300	1.21753300
H	-3.69092000	-0.38421800	-2.71836600
H	-5.30438800	-1.42471600	-1.14181900
C	1.21566500	-1.33130300	0.07942100
C	2.52127000	-1.36395600	0.59262400
C	0.85157100	-2.29657900	-0.86939500
C	3.43730300	-2.31876800	0.16156200
H	2.82290200	-0.63600300	1.34653900
C	1.76531900	-3.25541300	-1.30285000
H	-0.15985100	-2.30464600	-1.27566400
C	3.05911900	-3.26616200	-0.78868300
H	4.44512100	-2.32801400	0.57049900
H	1.46437700	-3.99721800	-2.03917900
H	3.77223800	-4.01597200	-1.12375500
C	0.48679800	1.68559800	-0.03844000
C	-0.39857500	2.76598000	0.11213100
C	1.72487400	1.91610000	-0.65432800
C	-0.06308600	4.03350100	-0.35278100
H	-1.36520900	2.60998300	0.59241000
C	2.06115400	3.18277400	-1.12410000
H	2.43031900	1.09485600	-0.77929900
C	1.16806400	4.24200900	-0.97251100
H	-0.76082300	4.85888400	-0.23227000

H	3.02055100	3.34407200	-1.61027300
H	1.43236400	5.23205600	-1.33697800

TS Ph₃SiS·-I₁



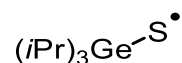
$$E = -1713.855048$$

$$G_{\text{Corr.}} = 0.433982$$

N	-3.63190000	0.13542600	-0.22152100
C	-2.39002000	-0.01008100	0.34269600
H	-2.03037000	0.84002800	0.92562400
H	-2.14658000	-0.99519500	0.74191100
C	-4.31791500	-1.04725900	-0.75923300
C	-4.86259000	-1.90771700	0.37405900
C	-3.43668300	-1.85848900	-1.70258500
H	-5.17033200	-0.66748700	-1.33804600
H	-5.52510000	-1.32608700	1.02520500
H	-5.42621100	-2.75776000	-0.02763700
H	-4.04565400	-2.30937000	0.98814800
H	-3.03542500	-1.23999000	-2.51329300
H	-2.58824800	-2.30776000	-1.17009000
H	-4.02042200	-2.67317700	-2.14645200
C	-4.05843800	1.47501800	-0.63952200
C	-5.50632100	1.74688800	-0.25832500
C	-3.79757100	1.72356100	-2.12066700
H	-3.42441000	2.16481800	-0.06299500
H	-5.67247600	1.56366600	0.80906100
H	-5.75735400	2.79176600	-0.47315100
H	-6.20544900	1.12214900	-0.82849700
H	-2.74049500	1.56282100	-2.36613900
H	-4.40449100	1.05875900	-2.74942100
H	-4.05811200	2.75558600	-2.38388100
Si	1.30788200	0.00628100	-0.23093100
S	-0.08067700	0.03479800	-1.86685100
H	-1.19059900	0.02717000	-0.90485100
C	2.99376900	-0.49825300	-0.88293100
C	3.59853800	0.25293500	-1.90218500
C	3.69526800	-1.59420100	-0.36529000
C	4.85460200	-0.08510700	-2.39598700
H	3.07705300	1.11648100	-2.31859500
C	4.95535800	-1.93669700	-0.85436200
H	3.25303500	-2.19262700	0.43150800
C	5.53520500	-1.18344000	-1.87124500
H	5.30481400	0.50777200	-3.18916000
H	5.48399100	-2.79246100	-0.43996900
H	6.51720100	-1.45021800	-2.25562400
C	1.43616400	1.70550100	0.56851300
C	2.49995700	1.98266400	1.44061200
C	0.48335000	2.70887700	0.35300200
C	2.60488500	3.21464600	2.08093900
H	3.26270500	1.22273400	1.62166000
C	0.58197300	3.94448400	0.99024100
H	-0.34200400	2.52483700	-0.33733900
C	1.64253000	4.19805300	1.85653600
H	3.43857100	3.40971600	2.75206400
H	-0.16656500	4.71222000	0.80594200
H	1.72342500	5.16276400	2.35257600
C	0.68658500	-1.23338300	1.04321700
C	0.36623900	-2.54192200	0.64786000
C	0.46403500	-0.87839700	2.37971900
C	-0.16150100	-3.45997300	1.55061600
H	0.51526100	-2.84151800	-0.39079800
C	-0.06495700	-1.79314000	3.29027600
H	0.69226100	0.13339800	2.71628800

C	-0.38149700	-3.08395600	2.87612800
H	-0.40543300	-4.46784600	1.22129400
H	-0.23564600	-1.49413700	4.32224600
H	-0.79893700	-3.79741700	3.58322200

(iPr)₃GeS·



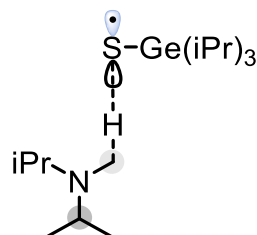
E =

G_{Corr.} =

S	0.58522100	-0.16499600	2.29279200
C	-1.95855000	-0.50696900	0.11290500
C	-2.43603600	-0.88688200	-1.28367100
C	-2.79231500	0.62312200	0.69734300
H	-2.03602900	-1.38622700	0.77054000
H	-1.86684900	-1.72071900	-1.71291700
H	-3.49440200	-1.18405900	-1.26893700
H	-2.35296900	-0.03891700	-1.97855300
H	-2.41989500	0.94481400	1.67836100
H	-2.78607400	1.49947600	0.03320200
H	-3.84182200	0.32025800	0.81901300
C	0.25522900	1.83854300	-0.35533200
C	0.18862300	1.98938000	-1.87074500
C	1.54551200	2.42068600	0.20671600
H	-0.59353600	2.37414200	0.09590400
H	-0.75177000	1.60820100	-2.29106000
H	0.27465200	3.04522900	-2.16539900
H	1.01115000	1.45050900	-2.36159300
H	1.58146000	2.36133700	1.30236300
H	2.43065900	1.89779600	-0.17939000
H	1.64606900	3.47926100	-0.07293900
C	0.99516000	-1.32597200	-0.90608000
C	0.76004700	-2.73063700	-0.36376700
C	2.47994200	-0.99168600	-0.90408200
H	0.61213300	-1.26689200	-1.93850400
H	-0.29986300	-3.01653400	-0.37001200
H	1.30710400	-3.47972500	-0.95366100
H	1.11706300	-2.80837500	0.67322300
H	2.69115300	-0.02030600	-1.36910000
H	2.87329700	-0.96156700	0.12208900
H	3.05572200	-1.75051400	-1.45329900
Ge	-0.05457700	-0.04014900	0.12300900

H	-5.80391700	-2.18551800	-0.64166900
H	-4.46646700	-2.64199700	0.42547500
H	-2.84241200	-0.59460700	-2.34207400
H	-2.86184800	-2.20380500	-1.59898600
H	-4.23749000	-1.67241200	-2.57795100
C	-3.22579000	1.26900000	0.55943400
C	-4.54675500	1.73693200	1.15341400
C	-2.85249200	2.05076300	-0.69539800
H	-2.43942700	1.43881000	1.31011200
H	-4.78584100	1.18095100	2.06681200
H	-4.48826100	2.80282500	1.40169800
H	-5.37794300	1.61279600	0.44746400
H	-1.89249200	1.70803200	-1.10234600
H	-3.61717500	1.94367800	-1.47601000
H	-2.76870700	3.11910500	-0.46056100
S	0.09683500	-0.53293300	-1.39863100
H	-0.93582000	-0.70518700	-0.32179000
C	1.49517500	-1.11794500	1.66226500
C	2.62215400	-0.88389800	2.66222800
C	1.33262200	-2.60010700	1.35906700
H	0.55663200	-0.74572000	2.10265600
H	2.77010000	0.18028100	2.89055600
H	2.42643400	-1.40119000	3.61278600
H	3.57520100	-1.27512700	2.27704900
H	0.51251500	-2.78803300	0.65503000
H	2.24684300	-3.01571300	0.91090700
H	1.13460600	-3.17576300	2.27538000
C	3.46036000	-0.61890300	-0.85168700
C	4.64111900	0.17281000	-0.29825700
C	3.40250400	-0.51386600	-2.36961400
H	3.58740700	-1.67907000	-0.57912100
H	4.71970600	0.11108300	0.79500600
H	5.59096600	-0.18933800	-0.71788900
H	4.56101300	1.23723100	-0.56021400
H	2.58929600	-1.11596300	-2.79147000
H	3.23971400	0.52434000	-2.69260400
H	4.34525000	-0.85219800	-2.82446500
C	1.77289900	1.84226300	0.44378100
C	0.54875800	2.21601300	1.26726300
C	1.84704100	2.68924800	-0.81906900
H	2.67827400	2.01931600	1.04753600
H	0.46833600	1.63666000	2.19713300
H	0.55896800	3.28119600	1.54135500
H	-0.36876000	2.04134500	0.68591100
H	2.75496200	2.49369400	-1.40440300
H	0.98605800	2.48791800	-1.47252000
H	1.83573800	3.76302600	-0.57973400
Ge	1.78608100	-0.07421400	0.02668300

TS (iPr)₃GeS·-I₁

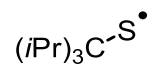


E =

G_{Corr.} =

C	-3.86468972	-2.29018737	-0.90627693
N	-3.22358100	-0.17995600	0.33423900
C	-2.13298100	-0.90991800	0.74330000
H	-1.64136600	-0.53939400	1.64605400
H	-2.23640800	-1.99447800	0.68354700
C	-4.17281300	-0.76132400	-0.62356600
C	-5.05971800	-1.79363000	0.06135300
C	-3.48437700	-1.33734200	-1.85542600
H	-4.81298500	0.06727800	-0.95463600
H	-5.58583500	-1.35316900	0.91601100

(iPr)₃CS·



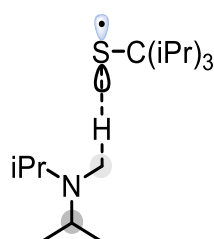
E = -791.6594977

G_{Corr.} = 0.250675

S	-0.24571600	0.35152300	1.92541600
C	1.56535100	0.40237900	-0.06206400
C	2.05846200	0.26334300	-1.50130300
C	2.51735900	-0.35790400	0.86247100
H	1.65610800	1.46098300	0.21681400
H	1.42945300	0.79085700	-2.22746100
H	3.06870600	0.68387200	-1.57677600
H	2.12459800	-0.78877000	-1.80643400
H	2.29189700	-0.19844000	1.92482400
H	2.51037200	-1.43964300	0.67911600
H	3.54344400	-0.00915000	0.69391000
C	-0.21044700	-1.46339400	-0.26023100
C	-0.60951900	-1.68803100	-1.72405500
C	-1.18929700	-2.23431800	0.62747400
H	0.75711900	-1.97049200	-0.12920000
H	0.03842900	-1.17480200	-2.44079200
H	-0.55309200	-2.76052000	-1.94651100

H	-1.64298100	-1.37587100	-1.92158200
H	-0.82828900	-2.32814200	1.65499600
H	-2.18037700	-1.76528800	0.66863300
H	-1.32258500	-3.24581600	0.22318200
C	-0.85830500	1.03499200	-0.66746200
C	-0.46412200	2.50627400	-0.55234900
C	-2.34025200	0.89854100	-0.31648200
H	-0.75254600	0.76210100	-1.72761800
H	0.51112700	2.72786300	-0.99860700
H	-1.20455600	3.11897400	-1.08061600
H	-0.44513100	2.83682500	0.49375300
H	-2.72218300	-0.11860400	-0.44457500
H	-2.53052700	1.19979800	0.72434200
H	-2.93863300	1.55669200	-0.95770800
C	0.05095400	0.04032000	0.12261000

TS (iPr)₃CS·-I₁



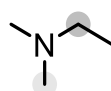
E = -1123.220647

G_{Corr.} = 0.460532

N	-2.90944600	-0.09012600	0.37560500
C	-1.74352000	-0.55660200	0.94369500
H	-1.41714900	-0.00268100	1.82747600
H	-1.66754600	-1.64267500	1.03511600
C	-3.64764500	-0.93812700	-0.56857500
C	-4.40271300	-2.03389400	0.17382000
C	-2.75707400	-1.51234300	-1.66418200
H	-4.38778000	-0.28396400	-1.04851400
H	-5.07426400	-1.60565600	0.92670000
H	-4.99902400	-2.63080800	-0.52606700
H	-3.70810800	-2.71402800	0.68314700
H	-2.22242200	-0.72277500	-2.20446800
H	-2.00927700	-2.20262200	-1.25330200
H	-3.36662300	-2.07145900	-2.38356900
C	-3.18036100	1.35091400	0.41023300
C	-4.62085500	1.63632100	0.81196200
C	-2.80221700	2.04331700	-0.89462200
H	-2.52710500	1.74298900	1.20355100
H	-4.86921000	1.14625000	1.75999400
H	-4.76801500	2.71580300	0.93116900
H	-5.33332300	1.29413900	0.05049700
H	-1.75084200	1.85678100	-1.14820900
H	-3.42751600	1.69379600	-1.72692500
H	-2.95055700	3.12603800	-0.80369300
S	0.52367600	-0.02304500	-1.07003500
H	-0.54657700	-0.28283300	-0.01087100
C	1.77395900	-1.10557300	1.15492800
C	2.83824500	-1.19166200	2.25279200
C	1.49934300	-2.52750000	0.66346400
H	0.85072700	-0.77484400	1.65007900
H	3.11059700	-0.22046100	2.68048300
H	2.45666000	-1.81370600	3.07251000
H	3.75433000	-1.67493400	1.89072100
H	0.77271300	-2.55345200	-0.15534300
H	2.41384800	-3.02962700	0.32132500
H	1.10245600	-3.12611000	1.49382400
C	3.27208400	-0.48090900	-0.84903500
C	4.63717700	-0.05432000	-0.29333800
C	3.23273500	-0.10856200	-2.33457600
H	3.25943400	-1.58076000	-0.83338700
H	4.76900000	-0.26732400	0.77088900
H	5.42598500	-0.59256700	-0.83355200
H	4.82328500	1.01667300	-0.44333200

H	2.38208800	-0.56197500	-2.85200900
H	3.18654400	0.97345400	-2.50162700
H	4.14778200	-0.47586900	-2.81729800
C	2.23456900	1.37049300	0.66068600
C	1.12591900	1.78279200	1.62844600
C	2.41317500	2.50236000	-0.34982300
H	3.16596900	1.32203000	1.24674700
H	1.01612100	1.10790000	2.48469600
H	1.34239700	2.78038200	2.02957700
H	0.15922200	1.83994700	1.10881600
H	3.28316000	2.36925700	-0.99898900
H	1.52571100	2.59883000	-0.98805900
H	2.55031900	3.45161200	0.18322400
C	2.04622700	-0.04423100	0.03245700

NEtMe₂

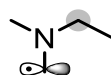


E = -213.686664

H_{Corr.} = 0.118215

N	0.45665100	-0.00296100	-0.34575800
C	-0.69783600	-0.65112700	0.26487300
H	-0.68238200	-1.70399600	-0.04908500
H	-0.59580600	-0.65256800	1.37375100
C	1.66283000	-0.75065900	-0.04890100
H	1.56835000	-1.77965100	-0.41430100
H	2.52410600	-0.28890300	-0.54480200
H	1.87550400	-0.79074300	1.04029900
C	0.60387600	1.37117900	0.09483400
H	1.50206900	1.80813100	-0.35531700
H	-0.25227600	1.97797400	-0.21606100
H	0.70144900	1.44674800	1.19895400
C	-2.02318500	-0.03029100	-0.13001900
H	-2.85262200	-0.64844900	0.22965500
H	-2.15778400	0.97117500	0.29353900
H	-2.10127300	0.04640000	-1.22104500

NEtMe₂I₁

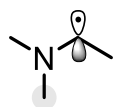


E = -213.029550

H_{Corr.} = 0.103418

N	0.52330700	-0.06449000	-0.17053700
C	-0.71818700	-0.61427400	0.35924300
H	-0.71714300	-1.68703700	0.12978700
H	-0.72385100	-0.52521800	1.46304200
C	1.64059200	-0.87525200	-0.08259300
H	1.48389500	-1.94454100	-0.19520700
H	2.59027600	-0.44166400	-0.38306100
C	0.73331500	1.34528500	0.08890100
H	1.67446300	1.66323200	-0.36938800
H	-0.07244400	1.94529400	-0.34482500
H	0.78493500	1.55606600	1.17239400
C	-1.95967100	0.03037500	-0.22507800
H	-2.85264900	-0.50553700	0.11316300
H	-2.07174500	1.07500900	0.08567200
H	-1.93517600	-0.00098600	-1.32066000

NEtMe₂I₂

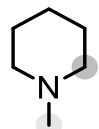


E = -213.031943

H_{Corr.} = 0.103496

N	0.45556700	-0.03126800	-0.24330700
C	-0.69506500	-0.72549700	0.12599600
H	-0.60772400	-1.80665000	0.02566500
C	0.50869100	1.38723700	0.04834700
H	1.39087700	1.82341500	-0.43184100
H	-0.37587500	1.89750500	-0.34314400
H	0.57210300	1.58288200	1.13558100
C	-2.03115100	-0.08967300	-0.00914200
H	-2.81365300	-0.81605900	0.23023100
H	-2.17090400	0.76893800	0.66365900
H	-2.22874000	0.27844700	-1.03341700
C	1.70563400	-0.71034800	0.02950300
H	1.63900900	-1.75401400	-0.29483100
H	2.52023800	-0.22908100	-0.52275800
H	1.95704600	-0.69682100	1.10577700

Me-pyperidine

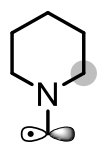


E = -291.077792

H_{Corr.} = 0.154896

C	-1.15067600	-1.24747900	-0.22619600
C	0.31474000	-1.20075300	0.17220100
C	0.31474300	1.20075000	0.17221200
C	-1.15066600	1.24748100	-0.22620500
C	-1.87776100	0.00000600	0.25965200
H	0.39717900	-1.24288000	1.28375700
H	0.85164900	-2.07529200	-0.21951100
H	-1.21834700	-1.31125400	-1.32252800
H	-1.61303600	-2.15597300	0.18079000
H	0.39717500	1.24285900	1.28376800
H	0.85166300	2.07529000	-0.21948300
H	-1.61303100	2.15598500	0.18075100
H	-1.21831700	1.31123400	-1.32254100
H	-1.89987300	0.00000900	1.36169900
H	-2.92219200	0.00000700	-0.07712600
N	0.96701400	0.00000000	-0.33383200
C	2.37452600	-0.00000100	0.00393900
H	2.86262900	-0.88826300	-0.41395400
H	2.86262800	0.88827000	-0.41393500
H	2.54334500	-0.00001400	1.10151900

Me-pyperidine I₁



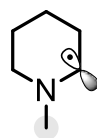
E = -290.420603

H_{Corr.} = 0.140606

C	1.08387200	1.24878100	-0.25846600
C	-0.34508400	1.22105900	0.25641400
C	-0.34508400	-1.22105900	0.25641400

C	1.08387200	-1.24878100	-0.25846600
C	1.83771900	0.00000000	0.18137000
H	-0.34669100	1.29615700	1.36344000
H	-0.91882200	2.07397200	-0.12624700
H	1.06854500	1.30304800	-1.35731400
H	1.58191900	2.15682300	0.10426300
H	-0.34669100	-1.29615700	1.36344000
H	-0.91882200	-2.07397200	-0.12624700
H	1.58191900	-2.15682300	0.10426300
H	1.06854500	-1.30304800	-1.35731400
H	1.93017100	0.00000000	1.27973800
H	2.85808400	0.00000000	-0.22157300
N	-1.02738000	0.00000000	-0.14994300
C	-2.40577000	0.00000000	-0.07800500
H	-2.91182000	0.93884000	-0.28620800
H	-2.91182000	-0.93884000	-0.28620800

Me-pyperidine I₂

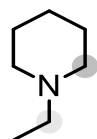


E = -290.422432

H_{Corr.} = 0.140366

C	-1.13357800	-1.21542300	-0.27099400
C	0.32935700	-1.20467700	0.13303200
C	0.29510200	1.21887300	0.09454700
C	-1.17419600	1.26801500	-0.14952400
C	-1.85787900	-0.01347300	0.31918700
H	0.41131600	-1.35887700	1.22991000
H	0.87726600	-2.02318300	-0.35203300
H	-1.20544400	-1.18587400	-1.36920000
H	-1.59010700	-2.15734400	0.05774200
H	0.88893500	2.12911600	0.01657600
H	-1.60094100	2.14923100	0.34544900
H	-1.38491500	1.39296600	-1.23196100
H	-1.81793000	-0.06933700	1.41832200
H	-2.91674200	-0.01534900	0.03151200
N	0.97995800	0.05037200	-0.22891400
C	2.39872100	0.05164600	0.05431700
H	2.87845400	-0.79812700	-0.44392400
H	2.85301100	0.97409800	-0.32195900
H	2.60222700	-0.01968800	1.13857400

Et-pyperidine



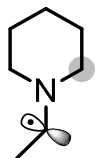
E = -330.371275

H_{Corr.} = 0.180962

C	-1.78811400	-1.04123400	-0.35270100
C	-0.38644800	-1.30431100	0.16988200
C	0.08200800	1.04119900	0.32449900
C	-1.30514000	1.39457900	-0.18678800
C	-2.30493200	0.29842600	0.15369200
H	-0.42284900	-1.41297200	1.27911200
H	0.00089200	-2.25144600	-0.22923800
H	-1.76208900	-1.03556100	-1.45272400
H	-2.45157900	-1.86100100	-0.04824500
H	0.07040100	1.01240500	1.43963800
H	0.79425300	1.82183500	0.03273800
H	-1.61498200	2.35754000	0.23936200
H	-1.25712400	1.52386000	-1.27847500

H	-2.43050900	0.24847900	1.24764000
H	-3.29272300	0.52344600	-0.26816500
N	0.53931700	-0.24023300	-0.20252900
C	1.88586600	-0.56617100	0.24998400
H	2.10133600	-1.58932700	-0.08818700
H	1.92550900	-0.59070700	1.36200500
C	2.95686900	0.36636600	-0.28345400
H	2.89440300	1.37135100	0.14816000
H	3.95087100	-0.02629500	-0.04328600
H	2.87831300	0.45690100	-1.37332400

Et-piperidine_I

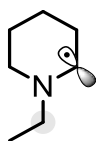


$$E = -329.716513$$

$$H_{\text{Corr.}} = 0.166446$$

C	1.78219300	-1.02230300	0.32185500
C	0.40809100	-1.32585400	-0.24882300
C	-0.14589000	1.03902900	-0.32965300
C	1.21918000	1.40366300	0.23095700
C	2.25748800	0.35122400	-0.13266300
H	0.47506800	-1.41577900	-1.35333600
H	0.03183800	-2.28427200	0.12994900
H	1.72981100	-1.05088300	1.42061100
H	2.48492800	-1.80549000	0.00988800
H	-0.11774600	1.07903200	-1.43991000
H	-0.89533200	1.76631100	-0.00027300
H	1.51048400	2.39178400	-0.14763700
H	1.14447800	1.48466200	1.32578700
H	2.39889800	0.34271500	-1.22578900
H	3.23120900	0.59490000	0.31039900
N	-0.55807200	-0.29168700	0.10241500
C	-1.89345700	-0.64748300	-0.07174900
H	-2.09334100	-1.70466500	0.09870500
C	-2.98165000	0.34000200	0.14951400
H	-2.99857800	1.14596100	-0.59887000
H	-3.95185300	-0.16348100	0.09863400
H	-2.91908600	0.83135400	1.13830600

Et-piperidine_I



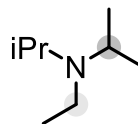
$$E = -329.715910$$

$$H_{\text{Corr.}} = 0.16626$$

C	1.77749100	-1.00613200	0.39009200
C	0.38707000	-1.31629400	-0.13295200
C	-0.07432000	1.05136400	-0.25335600
C	1.32458100	1.41817500	0.10761300
C	2.29880300	0.28932200	-0.21466300
H	0.44258500	-1.53116200	-1.22107100
H	-0.02092800	-2.21075200	0.35539300
H	1.73756900	-0.91080100	1.48622500
H	2.44189200	-1.84928700	0.16275000
H	-0.82938200	1.83163400	-0.31255800
H	1.60534200	2.34489200	-0.40798900
H	1.39976200	1.63688300	1.19307700
H	2.37823300	0.17428300	-1.30700400
H	3.30270500	0.52212000	0.16233100

N	-0.54237100	-0.21234200	0.09812300
C	-2.95368500	0.38975800	0.28280100
H	-2.89886300	1.40165200	-0.13228900
H	-3.95518800	0.00430000	0.06422400
H	-2.84202700	0.45964500	1.37109500
C	-1.90674900	-0.53805200	-0.30195100
H	-2.10184600	-1.56255100	0.04110200
H	-1.98240900	-0.55331100	-1.40764000

NEt(iPr)₂

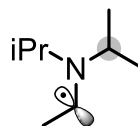


$$E = -370.859482$$

$$H_{\text{Corr.}} = 0.222521$$

N	-0.01030600	0.26664800	0.15228900
C	-0.39931500	1.40802600	-0.66088400
H	-1.48929700	1.39264200	-0.78522300
H	0.01771800	1.34627700	-1.68682600
C	1.40635500	-0.09178200	0.04873900
C	1.76526300	-0.99972400	-1.12901100
C	1.92363500	-0.67100400	1.35913300
H	1.93450600	0.86157500	-0.10722400
H	1.40279200	-0.59240400	-2.08101100
H	2.85410900	-1.10945000	-1.20669600
H	1.34365100	-2.00587500	-1.00271600
H	1.71133000	0.01112000	2.19028500
H	1.45789500	-1.63902100	1.58719300
H	3.00675700	-0.83730700	1.30836200
C	-0.97321700	-0.83722200	0.22124600
C	-1.58547500	-1.27053200	-1.11401500
C	-2.06952400	-0.50537800	1.22711800
H	-0.41924600	-1.70041600	0.61864500
H	-0.82191500	-1.47124700	-1.87319600
H	-2.17372200	-2.18629800	-0.97625700
H	-2.26702900	-0.50838800	-1.51345200
H	-1.63686700	-0.31496400	2.21600500
H	-2.62045000	0.39529400	0.92209100
H	-2.79530800	-1.32439100	1.31068000
C	-0.01445200	2.73310800	-0.02281400
H	1.06646300	2.80666400	0.14821400
H	-0.30583300	3.57655900	-0.66038000
H	-0.51302800	2.84014300	0.94841500

NEt(iPr)₂_I



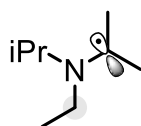
$$E = -370.209413$$

$$H_{\text{Corr.}} = 0.2081$$

N	0.01600000	0.23155900	0.22770900
C	0.08725300	1.59706500	-0.03512000
H	-0.87255600	2.10913800	-0.01960800
C	1.23744100	-0.57201000	0.11632500
C	1.52966400	-1.00560400	-1.31777700
C	1.23337800	-1.75568000	1.07436000
H	2.05343700	0.08679000	0.43996200
H	1.54020800	-0.13778500	-1.98928400
H	2.50448200	-1.50472600	-1.38153000
H	0.77155800	-1.71237300	-1.68150100
H	0.99552600	-1.43162500	2.09403700
H	0.51224600	-2.52957700	0.78264800

H	2.22298400	-2.22751700	1.08342100
C	-1.26693200	-0.43571200	-0.03503700
C	-1.89471100	-0.06988900	-1.37878400
C	-2.24001000	-0.19141100	1.11215700
H	-1.05268300	-1.51216900	-0.06190000
H	-1.17782800	-0.18115800	-2.19994200
H	-2.75254000	-0.72382100	-1.57724100
H	-2.25841100	0.96448300	-1.38810200
H	-1.81523700	-0.53770800	2.06147400
H	-2.46603100	0.87806000	1.21199800
H	-3.18620700	-0.71869600	0.93910300
C	1.30630600	2.38507100	0.28994500
H	2.17417400	2.13423000	-0.34007700
H	1.10296600	3.44973200	0.13727000
H	1.63757300	2.26282900	1.33890500

NEt(iPr)₂I₂

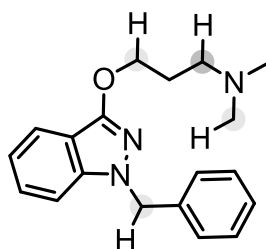


E = -370.205607

H_{Corr.} = 0.206858

N	-0.29638700	0.22939400	-0.20477600
C	-0.44269900	-1.14369100	0.33826700
C	0.42466200	-1.36434800	1.57230600
C	-0.21860300	-2.22094200	-0.71251400
H	-1.49415000	-1.22123500	0.65315800
H	0.23634400	-0.59489500	2.33191200
H	0.21982900	-2.34363400	2.02184100
H	1.49179800	-1.33130700	1.31449000
H	-0.83174500	-2.02518200	-1.60034300
H	0.83049300	-2.27328100	-1.02582800
H	-0.49238200	-3.20430200	-0.31012000
C	0.99979300	0.76339900	-0.32161700
C	1.55563500	1.73900100	0.66667000
C	1.96586600	0.13427500	-1.26412700
H	0.79554800	2.14843300	1.34064000
H	2.32457100	1.26127300	1.30425500
H	2.05847300	2.58385900	0.17224800
H	1.45905400	-0.29896700	-2.13433300
H	2.68539500	0.88444500	-1.62373600
H	2.57587200	-0.66668000	-0.80271000
C	-2.65901000	0.90203200	-0.46722400
H	-3.03554800	-0.11560300	-0.30695000
H	-3.42724300	1.59780900	-0.10943600
H	-2.53498900	1.04539000	-1.54680000
C	-1.34058600	1.14119800	0.25002000
H	-1.00735500	2.16421500	0.03799400
H	-1.48961100	1.07837000	1.34647800

Benzylamine



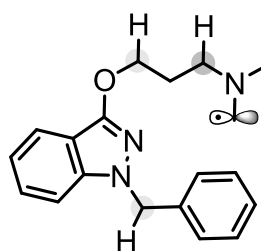
E = -976.895668

H_{Corr.} = 0.410364

O	-1.60801300	1.06745000	0.01901800
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N	1.55479400	0.31126900	-1.10705400
N	0.23037600	-0.01654400	-0.94976000
C	-0.31144600	0.99058400	-0.30141200
C	0.64060500	2.00490100	0.01824100
C	1.84667300	1.50415000	-0.51129500
C	3.19255200	-1.45721000	-0.51216400
C	-2.42170700	-0.03823800	-0.37723600
H	-2.02611800	-0.95884400	0.07848700
H	-2.35911300	-0.15904800	-1.46887300
C	2.73057800	-1.47942500	0.80364900
H	1.84561100	-0.90645500	1.07612900
C	2.48147200	-0.67856100	-1.59443600
H	3.21613900	-0.18145500	-2.24343800
H	1.90262300	-1.35381000	-2.23648400
C	1.79395200	3.94114500	0.79879300
H	1.80600200	4.90268100	1.30547800
C	3.39640400	-2.23003200	1.77061000
H	3.02750900	-2.23726400	2.79369700
C	4.33240900	-2.19296700	-0.84433300
H	4.70319100	-2.17286400	-1.86927300
C	-3.83442900	0.24184800	0.07283900
H	-3.82027700	0.45603500	1.14982600
H	-4.21624100	1.13850100	-0.43458300
C	-4.73761000	-0.93989700	-0.23869200
H	-4.57998700	-1.24717200	-1.28378800
H	-4.44228600	-1.80982200	0.39228000
C	3.05420000	2.20459700	-0.37734000
H	3.99077800	1.80971600	-0.76417600
C	4.52859600	-2.96615800	1.43226800
H	5.04755700	-3.55030000	2.18848900
C	0.60735500	3.24119500	0.67522900
H	-0.32526900	3.63055600	1.07674100
C	3.00045200	3.42111700	0.27985000
H	3.91640600	3.99418500	0.40476100
C	4.99614300	-2.94586300	0.11929700
H	5.88323100	-3.51301000	-0.15343000
N	-6.15426400	-0.65031300	-0.07984300
C	-6.94622200	-1.77448400	-0.54191700
H	-6.75489200	-2.69457300	0.04891500
H	-6.71779200	-1.99031200	-1.59183800
H	-8.01333000	-1.53804800	-0.46534400
C	-6.49289300	-0.33453700	1.29567700
H	-7.57230300	-0.16736100	1.37860100
H	-5.98932100	0.57991100	1.62482500
H	-6.21685700	-1.15472700	1.99169300

Benzylamine I₁



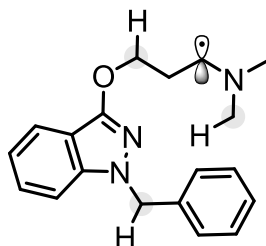
E = -976.238166

H_{Corr.} = 0.397017

O	-1.66536000	1.00675100	0.02336600
N	1.50969700	0.31028600	-1.10634800
N	0.19232300	-0.04209900	-0.94640100
C	-0.36730800	0.95559700	-0.29892500
C	0.56523600	1.98851900	0.01746100
C	1.77975300	1.50965800	-0.51329300
C	3.18161900	-1.42669000	-0.51366600
C	-2.45454800	-0.11725500	-0.36760300
H	-2.03894100	-1.02788500	0.09008300
H	-2.39269100	-0.24074900	-1.45899800
C	2.72722500	-1.45063300	0.80471700
H	1.83548500	-0.88959400	1.08003900
C	2.45396800	-0.66224500	-1.59504600

H	3.17774300	-0.15152400	-2.24568200
H	1.88682200	-1.34857200	-2.23574900
C	1.68365300	3.94685800	0.79368500
H	1.67866000	4.90907000	1.29917700
C	3.40931900	-2.18766800	1.77081200
H	3.04622200	-2.19641100	2.79594800
C	4.33019900	-2.14708700	-0.84947800
H	4.69491600	-2.12564600	-1.87655800
C	-3.87156300	0.13559900	0.08605700
H	-3.85883800	0.34522100	1.16392700
H	-4.26963300	1.02781500	-0.41653200
C	-4.75065700	-1.06388500	-0.22695200
H	-4.62806000	-1.34005500	-1.28340900
H	-4.42237400	-1.93835600	0.37006600
C	2.97429400	2.23253900	-0.38202400
H	3.91749800	1.85442600	-0.76949500
C	4.55028700	-2.90838700	1.42893900
H	5.08194400	-3.48191800	2.18444800
C	0.51007800	3.22501900	0.67291800
H	-0.42883100	3.59768500	1.07560600
C	2.89890000	3.44864300	0.27363700
H	3.80420500	4.03875700	0.39659300
C	5.01018900	-2.88638800	0.11328100
H	5.90388500	-3.44164900	-0.16226800
N	-6.16627500	-0.81464900	-0.00848400
C	-7.04451800	-1.63456800	-0.69569200
H	-6.74445100	-1.95510000	-1.68949900
H	-8.10073100	-1.52539300	-0.46699800
C	-6.53017500	-0.48398800	1.35517900
H	-7.60857100	-0.30947400	1.40980300
H	-6.02418900	0.42907400	1.68357900
H	-6.27310000	-1.30033100	2.05358200

Benzylamine I₂



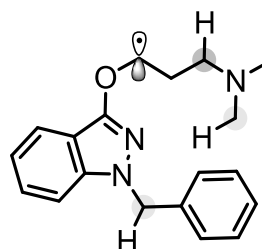
E = -976.240946

H_{Corr.} = 0.397041

O	-1.64271500	1.05973600	0.01280400
N	1.52121900	0.30317600	-1.10936600
N	0.19668800	-0.02519700	-0.95277800
C	-0.34627400	0.98244000	-0.30608200
C	0.60527900	1.99754700	0.01326700
C	1.81207700	1.49668200	-0.51446300
C	3.16382500	-1.45739000	-0.50578600
C	-2.45515400	-0.04942000	-0.37562200
H	-2.06524300	-0.96763900	0.08702600
H	-2.39582400	-0.17649900	-1.46655900
C	2.69274400	-1.48623500	0.80675800
H	1.79854700	-0.92474800	1.07296800
C	2.44930100	-0.68770600	-1.59215200
H	3.18186500	-0.19363400	-2.24585000
H	1.87023600	-1.36827700	-2.22834800
C	1.75727400	3.93498400	0.79315200
H	1.76845900	4.89696600	1.29904000
C	3.36104500	-2.22890800	1.77800100
H	2.98490500	-2.24157100	2.79839000
C	4.31531300	-2.17821300	-0.83015900
H	4.69334000	-2.15247800	-1.85231500
C	-3.86862500	0.23591100	0.07336900
H	-3.85658200	0.41616400	1.16025400
H	-4.19957000	1.18778100	-0.38691200
C	-4.76359800	-0.89689500	-0.29077600

H	-4.49043100	-1.52489200	-1.14052700
C	3.01922600	2.19767000	-0.37992600
H	3.95632700	1.80263000	-0.76536000
C	4.50486800	-2.95052600	1.44731200
H	5.02569900	-3.52857100	2.20693700
C	0.57102000	3.23442500	0.66896000
H	-0.36212800	3.62375900	1.06930500
C	2.96446600	3.41487200	0.27599700
H	3.88013700	3.98831200	0.40135600
C	4.98157700	-2.92341800	0.13782800
H	5.87781000	-3.47898600	-0.12879500
N	-6.13292000	-0.81568700	-0.06368400
C	-6.58181300	-0.14782300	1.14185900
H	-7.66944900	-0.02846600	1.10472000
H	-6.13630300	0.84767300	1.22341300
H	-6.32529700	-0.72222100	2.05142300
C	-6.88659700	-2.01643700	-0.36379000
H	-7.95460000	-1.78047600	-0.42271900
H	-6.56905300	-2.42125300	-1.33015900
H	-6.74175300	-2.79687300	0.40461300

Benzylamine I₃

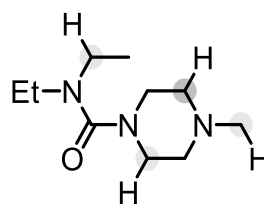


E = -976.232079

H_{Corr.} = 0.396224

O	-1.62281500	1.14168800	-0.01936100
N	1.53555900	0.31341500	-1.11029800
N	0.20448600	0.01771400	-0.97679700
C	-0.31723600	1.03353500	-0.32765500
C	0.64808300	2.02344700	0.01282600
C	1.84898500	1.49625500	-0.50388200
C	3.14347500	-1.48160800	-0.52268500
C	-2.47902700	0.13262500	-0.37301200
H	-2.03004100	-0.83022300	-0.60801800
C	2.65205800	-1.53532200	0.78169800
H	1.75544700	-0.97654000	1.04590500
C	2.44566600	-0.69011100	-1.60390200
H	3.18732900	-0.20281400	-2.25214200
H	1.85320800	-1.35262500	-2.24655300
C	1.83957500	3.92368100	0.82219400
H	1.86912900	4.88101200	1.33599500
C	3.30325900	-2.29939500	1.74778400
H	2.91150600	-2.33158800	2.76181600
C	4.29819700	-2.19838400	-0.84397500
H	4.69231200	-2.15274500	-1.85926300
C	-3.86431800	0.31374700	0.10798100
H	-3.86167200	0.45228300	1.20438900
H	-4.30209200	1.23560600	-0.30973000
C	3.07180100	2.16490400	-0.34997800
H	4.00281600	1.74906400	-0.72795600
C	4.45019000	-3.01746400	1.41996500
H	4.95777300	-3.61222400	2.17559800
C	0.63726900	3.25560800	0.67920100
H	-0.28994700	3.66592500	1.07197800
C	3.03972800	3.37783300	0.31480300
H	3.96763800	3.92732200	0.45553800
C	4.94733100	-2.96506400	0.11897000
H	5.84633700	-3.51738700	-0.14489000
N	-6.15099700	-0.65456800	-0.06445000
C	-6.46685000	-0.48281800	1.34169100
H	-7.54930200	-0.36597300	1.46277000
H	-5.98939100	0.41561600	1.74570700

H	-6.14373400	-1.35326800	1.95082700
C	-6.91447900	-1.75847600	-0.61504800
H	-7.98689600	-1.57044400	-0.49251400
H	-6.70525500	-1.86444100	-1.68550100
H	-6.67587700	-2.72277400	-0.11973600
C	-4.73058700	-0.87371900	-0.28310600
H	-4.38292300	-1.78089800	0.26215300
H	-4.58590700	-1.07796100	-1.35389500

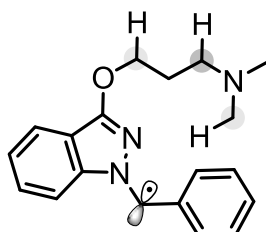


$$E = -632.953165$$

$$H_{\text{Corr.}} = 0.32961$$

O	0.48507200	-1.93854400	-0.65798400
N	1.82739400	-0.14260500	-0.23323500
N	-0.37430300	0.15596400	-1.01889500
N	-2.92100400	0.41863600	0.27907500
C	2.88810600	2.06346300	0.20912100
H	2.10277100	2.37446700	0.90887100
H	3.28462600	2.95924000	-0.28107800
H	3.69999800	1.62428900	0.80106500
C	2.36312600	1.08289500	-0.82453300
H	3.17813800	0.80635500	-1.51369800
H	1.58661300	1.54165400	-1.44318200
C	0.63771300	-0.71719000	-0.63417100
C	-0.70117500	1.33317300	-0.21385700
H	-1.11508700	2.10427400	-0.87978900
H	0.19715500	1.73787100	0.25515600
C	-1.71393000	0.98123900	0.86162400
H	-1.24351500	0.26393900	1.57474400
H	-1.97971000	1.88262300	1.43029300
C	-3.90014300	0.12162800	1.30451500
H	-3.52939000	-0.62725800	2.03390400
H	-4.81373400	-0.27338500	0.84569100
H	-4.15814400	1.03485400	1.85327300
C	-2.59585000	-0.77633600	-0.49137000
H	-3.51742200	-1.16151600	-0.94779500
H	-2.18836400	-1.57199400	0.16757600
C	-1.58111600	-0.45322600	-1.57250100
H	-1.30270100	-1.35694100	-2.11881200
H	-2.01777800	0.26640800	-2.27975100
C	2.80687200	-1.05211300	0.36512400
H	3.79356500	-0.58739100	0.25328900
H	2.82374500	-1.99182000	-0.20005200
C	2.51198800	-1.31544900	1.82996100
H	2.52028000	-0.37915600	2.40210100
H	3.25537900	-1.99302800	2.26484700
H	1.52485000	-1.77760300	1.94512100

Benzylamine I4



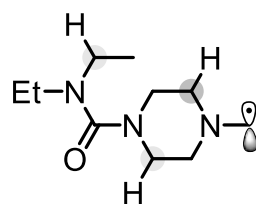
$$E = -976.256496$$

$$H_{\text{Corr.}} = 0.397174$$

O	-1.34665400	1.37601600	-0.07045300
N	1.99142100	0.55964200	0.00194300
N	0.66628100	0.19544100	-0.02216300
C	-0.01670500	1.31879000	-0.04354700
C	0.82353400	2.47288500	-0.03450200
C	2.12333500	1.93856500	-0.00463400
C	2.97986100	-1.75570700	0.03080100
C	1.81001800	-2.56198000	0.00208700
H	0.83659300	-2.08509800	-0.02315800
C	3.02706600	-0.34238000	0.02931900
H	4.00040600	0.13984400	0.05123500
C	1.72966100	4.67633200	-0.03219400
H	1.60772100	5.75618800	-0.04263300
C	1.91009000	-3.94527700	0.00579300
H	0.99874700	-4.53951600	-0.01692000
C	4.23412400	-2.42786800	0.06368800
H	5.14648100	-1.83293700	0.08635000
C	-3.51822500	0.41427900	-0.10934200
H	-3.75583200	1.08857700	0.72412300
H	-3.77509400	0.93923300	-1.03968000
C	3.25319300	2.76304400	0.01206000
H	4.26363700	2.36404000	0.03490300
C	3.15157800	-4.58431800	0.03795600
H	3.21335800	-5.66970300	0.04043200
C	0.61551600	3.85521600	-0.04871200
H	-0.39183100	4.26347300	-0.07239700
C	3.02987500	4.13016800	-0.00208400
H	3.88417300	4.80276600	0.01018000
C	4.31529500	-3.80735000	0.06703600
H	5.29114100	-4.28742600	0.09243300
N	-5.73452100	-0.70101700	-0.30430900
C	-6.38464600	0.15891300	0.66766200
H	-7.45435300	0.22476900	0.44137600
H	-5.97528300	1.17347800	0.63160000
H	-6.27462700	-0.22529900	1.70372000
C	-6.39436900	-1.99238100	-0.34719300
H	-7.45052400	-1.86493100	-0.60923500
H	-5.92746900	-2.62915600	-1.10715900
H	-6.34345800	-2.52301300	0.62641800
C	-4.31927800	-0.87389900	-0.01717600
H	-4.17575700	-1.32943900	0.98975400
H	-3.92178200	-1.59766700	-0.74489600
C	-2.03871500	0.12178300	-0.07798300
H	-1.75519300	-0.44846800	0.81951000
H	-1.71732900	-0.45918900	-0.95483200

Diethylcarbamazine

Diethylcarbamazine I1



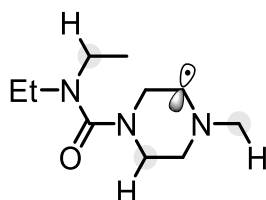
$$E = -632.294933$$

$$H_{\text{Corr.}} = 0.316117$$

O	0.44178100	-1.97532300	-0.51259400
N	1.79174100	-0.15533100	-0.24637300
N	-0.42974800	0.08970700	-0.99513000
N	-2.90445100	0.34080800	0.39551100
C	2.84292200	2.08052500	0.04600800
H	2.07232000	2.42368300	0.74711400
H	3.21802800	2.95053300	-0.50366500
H	3.67359100	1.68238100	0.64076600
C	2.30303900	1.03897800	-0.91789400
H	3.10479800	0.72927000	-1.60828200

H	1.50912000	1.45556300	-1.54424000
C	0.59535400	-0.75590600	-0.57578300
C	-0.75092000	1.30594900	-0.24833800
H	-1.20906300	2.02550200	-0.94220100
H	0.15522000	1.75898500	0.15733100
C	-1.70789700	0.99900600	0.89104400
H	-1.19409400	0.35546700	1.63561200
H	-2.00136900	1.92647400	1.39798400
C	-3.99849300	0.30860800	1.23843000
H	-4.85192500	-0.28114500	0.91600900
H	-4.15121300	1.16982500	1.88314500
C	-2.61573600	-0.86851100	-0.36530000
H	-3.55741500	-1.25294200	-0.77559600
H	-2.18861800	-1.64406000	0.29628900
C	-1.64063900	-0.56193400	-1.48777200
H	-1.36256800	-1.48084600	-2.00838800
H	-2.11080100	0.12236900	-2.20829000
C	2.79063900	-1.01901900	0.38745200
H	3.77299000	-0.56610000	0.20854400
H	2.78894700	-1.99806100	-0.10638300
C	2.54273900	-1.17190300	1.87648500
H	2.56685800	-0.19575400	2.37695800
H	3.30109800	-1.81511500	2.33676100
H	1.56100700	-1.62448400	2.05722500

Diethylcarbamazine_I₂

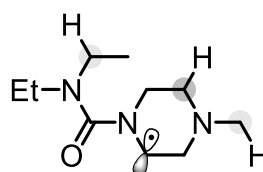


$$E = -632.296589$$

$$H_{\text{Corr.}} = 0.31644$$

O	0.40651200	-1.88631600	-0.72302100
N	1.80048700	-0.14680300	-0.24110300
N	-0.38711100	0.24282900	-1.02641300
N	-2.86338700	0.34347700	0.39851900
C	2.88276700	2.01314600	0.34887400
H	2.09799000	2.28089900	1.06687200
H	3.28629500	2.93710000	-0.07940600
H	3.69030800	1.52907000	0.91099200
C	2.35308800	1.10752100	-0.74896800
H	3.16978500	0.86576200	-1.44906600
H	1.58682300	1.61408200	-1.34243500
C	0.59564500	-0.67110600	-0.65755000
C	-0.70702300	1.39605100	-0.17523600
H	-1.03109300	2.21219200	-0.85278100
H	0.18471300	1.75325000	0.34326000
C	-1.75528100	1.05955800	0.82981300
H	-1.93251300	1.74767100	1.65497000
C	-2.58664700	-0.75505100	-0.52275100
H	-3.53293600	-1.06984300	-0.98155300
H	-2.16957400	-1.61620100	0.03050200
C	-1.60499500	-0.32237600	-1.59572900
H	-1.34559700	-1.17235000	-2.23070400
H	-2.06177600	0.45627700	-2.22383100
C	2.76524500	-1.10429300	0.30358100
H	3.76194700	-0.66111600	0.19070500
H	2.74589800	-2.01962300	-0.30009600
C	2.49139600	-1.42231500	1.76162500
H	2.53933900	-0.51348700	2.37412800
H	3.22277000	-2.14014600	2.14990800
H	1.49302700	-1.85886000	1.87701900
C	-3.84648700	0.01263900	1.40821600
H	-4.07582000	0.89972700	2.00749600
H	-4.76919900	-0.32873100	0.92656200
H	-3.48865900	-0.78430300	2.08335000

Diethylcarbamazine_I₃

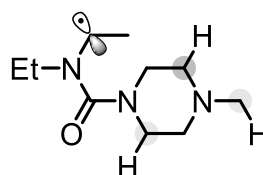


$$E = -632.293428$$

$$H_{\text{Corr.}} = 0.316191$$

O	1.11996000	-2.10614000	-0.29199900
N	1.91923200	0.03906300	-0.22496000
N	-0.40771700	-0.41336900	-0.21681600
N	-3.14114000	0.33657600	-0.11312600
C	2.37171000	2.48162200	-0.26061600
H	1.73253800	2.68707700	0.60634600
H	2.36820200	3.36742500	-0.90496600
H	3.39523100	2.34414700	0.10825900
C	1.88651900	1.26708600	-1.02875800
H	2.51482300	1.11007900	-1.92015900
H	0.86651400	1.42994600	-1.38957400
C	0.90332300	-0.89494200	-0.26488600
C	-0.76744700	0.84648600	0.24801800
H	0.01151400	1.38281900	0.78126100
C	-2.77269900	-1.06835200	-0.07594900
H	-3.54228400	-1.65713900	-0.59032700
H	-2.71802200	-1.43461500	0.97307800
C	-1.45076800	-1.27985300	-0.77368000
H	-1.11374800	-2.31347200	-0.67226000
H	-1.56802500	-1.05194100	-1.84369700
C	3.25843500	-0.51013200	0.01788600
H	3.98110900	0.22421100	-0.35527700
H	3.39071900	-1.42580700	-0.57219900
C	3.50358900	-0.77898300	1.48955700
H	3.40158200	0.14464600	2.07279300
H	4.51110100	-1.17913600	1.64897900
H	2.78524400	-1.51027000	1.87575500
C	-4.48203700	0.54638800	0.39366200
H	-4.73512800	1.61177300	0.35035300
H	-5.20368900	-0.00322800	-0.22063700
H	-4.59126500	0.20876800	1.44465500
C	-2.17502700	1.08895300	0.66840100
H	-2.29135300	0.82646700	1.75282200
H	-2.40095600	2.16185100	0.59329200

Diethylcarbamazine_I₄



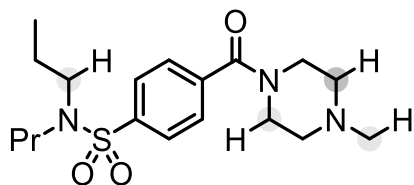
$$E = -632.299170$$

$$H_{\text{Corr.}} = 0.315758$$

O	0.47556600	-2.04882500	-0.50486800
N	1.85513400	-0.23406400	-0.29600300
N	-0.35988100	0.02140400	-1.04678400
N	-2.87696300	0.49951200	0.24354400
C	3.16636100	1.90110900	-0.19468500
H	2.65019100	2.36988800	0.66456300
H	3.47018000	2.70512900	-0.87101400
H	4.08315700	1.44987900	0.20988700
C	2.29595700	0.93559700	-0.90925100
H	1.75085000	1.22756500	-1.80185500
C	0.63456000	-0.83227200	-0.59711600

C	-2.59648600	-0.78040100	-0.39609200
H	-3.53475700	-1.18799400	-0.79498900
H	-2.19822300	-1.51071400	0.34005600
C	-1.59162100	-0.60559400	-1.52011100
H	-1.34658000	-1.56964800	-1.97087000
H	-2.01733100	0.04931400	-2.29343700
C	2.76192400	-1.00682200	0.56239100
H	3.78194500	-0.67211900	0.35141100
H	2.69342300	-2.05583300	0.25802400
C	2.41797900	-0.84801500	2.03091300
H	2.47065200	0.20418300	2.33756800
H	3.10786300	-1.42337600	2.65799200
H	1.40155400	-1.21014900	2.22779000
C	-3.85014500	0.34362100	1.30533400
H	-4.07461200	1.31770000	1.75505200
H	-4.78059200	-0.07133400	0.90142400
H	-3.49068100	-0.33319000	2.10722400
C	-1.64642900	1.08533800	0.74878600
H	-1.18892700	0.43590800	1.53169600
H	-1.87839100	2.05064400	1.21860900
C	-0.63819300	1.28988600	-0.36743600
H	-1.03822200	1.99516000	-1.10984500
H	0.28250000	1.71693700	0.03795800

Probenedicid derivative (38)



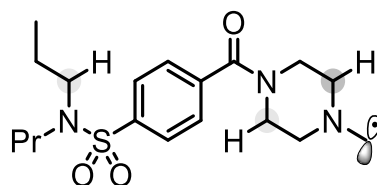
E = -1491.069206

H_{Corr.} = 0.487648

S	2.60713300	0.49358900	-1.39566000
O	-2.72290000	-2.31351800	1.48481600
O	3.00659800	-0.37170400	-2.49999600
O	2.54308300	1.94138300	-1.56284400
N	3.66020500	0.20704200	-0.14209600
C	-2.76198300	-1.41783000	0.64313000
C	-1.47732900	-0.90288900	0.06568500
C	-1.13785800	0.44990300	0.13036900
H	-1.84406300	1.16762100	0.54403000
C	0.10362700	0.88403400	-0.32039600
H	0.37420400	1.93605900	-0.28542400
C	0.99376200	-0.04618300	-0.85151100
C	0.66809900	-1.39996500	-0.92648200
H	1.36588400	-2.10834300	-1.36576000
C	-0.56473300	-1.82537200	-0.44972300
H	-0.83139900	-2.87895600	-0.47960500
C	3.54866900	1.10077700	1.02316200
H	3.59718500	0.47246200	1.92509900
H	2.55869100	1.57989000	1.04487400
C	4.62990700	2.16681500	1.05394100
H	4.54100300	2.77707800	0.14601300
H	5.61484500	1.68126600	1.00968100
C	4.51662900	3.03137700	2.29854900
H	5.29100700	3.80465000	2.32216700
H	4.61916000	2.43047900	3.21165500
H	3.54290900	3.53590400	2.34312700
H	5.74635600	-3.35137800	-0.03806600
C	4.03058700	-1.18654400	0.13264600
H	3.92690300	-1.75454100	-0.79882900
H	3.33640100	-1.62345100	0.87420600
C	5.46249700	-1.30370400	0.62764000
H	5.58948900	-0.72260200	1.55244100
H	6.12978100	-0.85405600	-0.12010500
C	5.83354500	-2.75615700	0.87940100
H	6.86296300	-2.84889000	1.23959100
H	5.17601800	-3.20923200	1.63207300

N	-3.92281500	-0.83145200	0.24020600
C	-4.11237000	-0.07012200	-0.99085200
C	-5.18144700	-1.22273900	0.86173200
H	-4.60908800	-0.71906500	-1.72972700
H	-3.14794600	0.23136200	-1.40463500
C	-6.04012100	0.00041600	1.09206500
H	-4.95755900	-1.73680000	1.80160800
H	-5.70759200	-1.93479800	0.20174200
N	-6.25865500	0.72994600	-0.14839800
H	-7.01257700	-0.30542600	1.49829800
H	-5.55135600	0.65121600	1.85009100
C	-7.12255400	1.87350100	0.06672600
H	-7.30261100	2.39057400	-0.88240300
H	-8.08771700	1.54253200	0.46599500
H	-6.68491500	2.60135500	0.77975900
C	-4.98692800	1.13787700	-0.72308400
H	-4.45143800	1.83943800	-0.04447800
H	-5.17604600	1.66899200	-1.66463800
C	1.21288679	5.66710896	0.00000000
C	-0.21606921	5.63938696	0.51488000
C	-0.21606921	3.19726896	0.51488000
C	1.21288679	3.16954696	0.00000000
C	1.96673379	4.41832796	0.43983600
H	-0.21767621	5.71448496	1.62190600
H	-0.78980721	6.49229996	0.13221900
H	1.19755979	5.72137596	-1.09884800
H	1.71093379	6.57515096	0.36272900
H	-0.21767621	3.12217096	1.62190600
H	-0.78980721	2.34435596	0.13221900
H	1.71093379	2.26150496	0.36272900
H	1.19755979	3.11527996	-1.09884800
H	2.05918579	4.41832796	1.53820400
H	2.98709879	4.41832796	0.03689300
N	-0.89836521	4.41832796	0.10852300
C	-2.27675521	4.41832796	0.18046100
H	-2.78280521	5.35716796	-0.02774200
H	-2.78280521	3.47948796	-0.02774200

Probenedicid₁₁



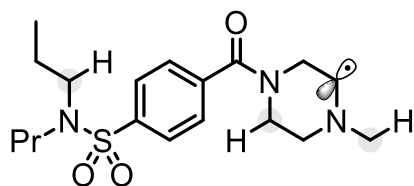
E = -1490.410538

H_{Corr.} = 0.474103

S	2.56963000	0.51566800	-1.38444200
O	-2.77944000	-2.30867700	1.45573400
O	2.95514100	-0.33168000	-2.50743700
O	2.51400500	1.96663500	-1.52400400
N	3.62797300	0.19803200	-0.14349300
C	-2.80712500	-1.39335000	0.63629600
C	-1.51880400	-0.87794700	0.06886400
C	-1.16900700	0.47081500	0.15794200
H	-1.86756000	1.18608900	0.58835400
C	0.07421100	0.90389600	-0.28907700
H	0.35270300	1.95305300	-0.23547000
C	0.95522100	-0.02286700	-0.84079200
C	0.61946700	-1.37269600	-0.93912700
H	1.31037000	-2.07791300	-1.39410000
C	-0.61482300	-1.79787900	-0.46605100
H	-0.88965000	-2.84864500	-0.51481400
C	3.53084600	1.06992600	1.03948500
H	3.57950200	0.42369900	1.92866800
H	2.54500100	1.55651800	1.07638400
C	4.62082700	2.12650900	1.08447700
H	4.53088300	2.75587200	0.18981800
H	5.60153600	1.63431400	1.02367300
C	4.52264900	2.96629000	2.34721100

H	5.30318200	3.73294200	2.38125800
H	4.62664400	2.34606100	3.24711100
H	3.55323300	3.47726900	2.40879700
H	5.69754800	-3.37121900	-0.13049700
C	3.99354900	-1.20252900	0.10083600
H	3.87864600	-1.75173300	-0.84051100
H	3.30355200	-1.65004000	0.83995100
C	5.42912300	-1.33679200	0.58067800
H	5.56709000	-0.77579000	1.51625800
H	6.09202600	-0.87480400	-0.16342900
C	5.79510700	-2.79597200	0.79860100
H	6.82697800	-2.90111600	1.14817900
H	5.14162100	-3.26182300	1.54698300
N	-3.96351900	-0.78420700	0.24766500
C	-4.14538400	-0.00140300	-0.97061600
C	-5.22586500	-1.18740200	0.85624500
H	-4.66317400	-0.62818800	-1.71426200
H	-3.17811700	0.28402600	-1.38909800
C	-6.06589900	0.04206000	1.14243500
H	-5.00783900	-1.73641200	1.77492000
H	-5.76265900	-1.86097500	0.16985700
N	-6.24257100	0.84186900	-0.06034900
H	-7.05377900	-0.26053700	1.50835300
H	-5.58239800	0.64633300	1.93385300
C	-7.24572600	1.79280400	-0.03925500
H	-7.30622600	2.46643800	-0.88919200
H	-8.14299100	1.55115800	0.52303700
C	-4.98436300	1.22636900	-0.67799100
H	-4.42521700	1.91533600	-0.01437200
H	-5.19985200	1.76031000	-1.61071300

Probeneid_I₂



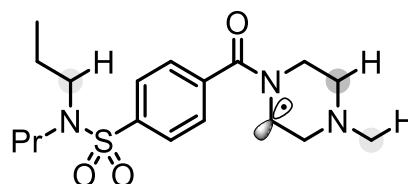
E = -1490.412828

H_{Corr.} = 0.474404

S	2.57482500	0.25865800	-1.46563600
O	-2.82680100	-2.28596200	1.49136500
O	3.07248400	-0.75614400	-2.38788100
O	2.49110600	1.65878200	-1.86668000
N	3.54302300	0.20927000	-0.11373200
C	-2.85298100	-1.50176900	0.54277800
C	-1.55791200	-1.03700600	-0.05244800
C	-1.25153300	0.32162100	-0.15684300
H	-1.99976400	1.06838900	0.111168900
C	0.00400600	0.72414000	-0.59835900
H	0.24878000	1.77846300	-0.69668100
C	0.94148400	-0.24484200	-0.94813800
C	0.64820700	-1.60502600	-0.85426500
H	1.38470700	-2.34608100	-1.15422900
C	-0.60014500	-1.99563400	-0.38890600
H	-0.84297300	-3.05027500	-0.28512900
C	3.33840300	1.28067100	0.87595900
H	3.31139400	0.81064800	1.87051800
H	2.35190900	1.74652400	0.73772700
C	4.41601700	2.34934000	0.81658600
H	4.40528700	2.79668400	-0.18561600
H	5.40028600	1.87554600	0.93684900
C	4.20047300	3.41008100	1.88306300
H	4.97263700	4.18480400	1.84058300
H	4.22332600	2.97302400	2.88993100
H	3.22814300	3.90397000	1.75954000
H	5.61823700	-3.24964900	0.75708000
C	3.89180200	-1.11389400	0.41829800
H	3.87259100	-1.82858200	-0.41231300
H	3.13548400	-1.43556700	1.15831000

C	5.27437800	-1.12501100	1.04862300
H	5.31842300	-0.39859400	1.87285400
H	6.00501800	-0.79364700	0.29832300
C	5.62319100	-2.51052600	1.56780500
H	6.61667400	-2.52676200	2.02693200
H	4.90185800	-2.84396600	2.32454700
N	-4.01140100	-1.01826200	0.02217300
C	-4.17175700	-0.17797400	-1.16206200
C	-5.26566200	-1.19066700	0.73850900
H	-4.82910400	-0.73722200	-1.85784000
H	-3.21738900	-0.04486500	-1.67602200
C	-4.76885000	1.13407200	-0.78448200
C	-5.75028100	0.16909400	1.20725600
H	-5.10176400	-1.86138000	1.58442200
H	-6.00246300	-1.64757400	0.06202100
N	-5.84195800	1.10978400	0.09608400
H	-4.77958300	1.93995500	-1.51616600
H	-6.74097000	0.08011100	1.66999500
H	-5.05111300	0.55792800	1.97370500
C	-6.40025000	2.39302400	0.46975000
H	-6.53063400	3.01328200	-0.42246000
H	-7.37997700	2.24719600	0.93688200
H	-5.74970700	2.93198500	1.17986900

Probeneid_I₃



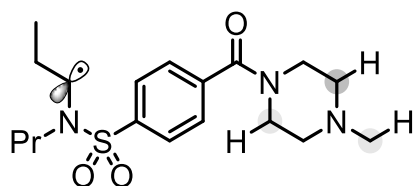
E = -1490.409741

H_{Corr.} = 0.473694

S	2.61091300	0.61601100	-1.35918700
O	-2.71567500	-2.31563000	1.40415100
O	2.95353100	-0.16064800	-2.54540600
O	2.58670200	2.07410400	-1.39891500
N	3.68893000	0.19111300	-0.16671900
C	-2.74397600	-1.32973600	0.67020400
C	-1.47428500	-0.79237900	0.09644900
C	-1.08450500	0.53719400	0.28210300
H	-1.74802100	1.23175300	0.79510100
C	0.15492700	0.97570100	-0.16863800
H	0.46067300	2.01066300	-0.04006500
C	0.99763300	0.07547400	-0.81650400
C	0.62573800	-1.25497300	-1.00730700
H	1.28655900	-1.93870600	-1.53410400
C	-0.60523000	-1.68733800	-0.53324100
H	-0.90690500	-2.72473900	-0.65453000
C	3.64279400	0.98721200	1.07153200
H	3.67058600	0.28387800	1.91740900
H	2.68106400	1.51461600	1.15117500
C	4.77944800	1.98980000	1.17000700
H	4.71078200	2.67677000	0.31684600
H	5.73716100	1.46046700	1.06870200
C	4.72886200	2.75343800	2.48287800
H	5.54383000	3.48053000	2.55608000
H	4.81104300	2.07462800	3.34179600
H	3.78422000	3.30278700	2.58553300
H	5.63225700	-3.43884000	-0.41736100
C	4.00839000	-1.23407400	-0.01790100
H	3.86500000	-1.71646300	-0.99140500
H	3.31071100	-1.70518500	0.69918900
C	5.44308100	-1.44980400	0.43400600
H	5.61025600	-0.96012500	1.40410300
H	6.11462400	-0.96121100	-0.28497000
C	5.75914000	-2.93237800	0.54751800
H	6.78991000	-3.09700900	0.87680300
H	5.09667000	-3.42529800	1.27023000
N	-3.92898200	-0.67154500	0.38843000

C	-4.09536300	0.20211500	-0.78696900
C	-5.08932600	-1.10654300	0.99909200
H	-4.34875600	-0.42688200	-1.65150800
H	-3.15836100	0.71630000	-1.00175500
C	-6.30538300	-0.25661300	0.96773500
H	-4.96446900	-1.88085700	1.74669800
N	-6.44656800	0.49919700	-0.26706900
H	-7.19521200	-0.88257700	1.11616700
H	-6.27785200	0.44920400	1.83797600
C	-5.20675800	1.19728200	-0.54972500
H	-4.92956200	1.88421400	0.28151600
H	-5.33471700	1.80743100	-1.45217800
C	-7.56728400	1.41385600	-0.18375800
H	-7.68713800	1.94481100	-1.13433200
H	-8.48863200	0.85556600	0.01596600
H	-7.43788200	2.16471700	0.62189200

Probenecid_{I4}



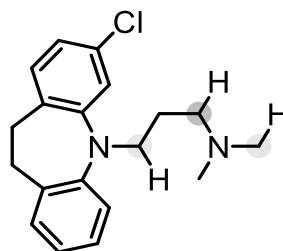
E = -1490.412331

H_{Corr.} = 0.473264

S	2.80697500	-1.67462700	0.33071900
O	-2.34083100	2.41995700	1.21761100
O	3.41197800	-1.93827400	1.63084800
O	2.68928700	-2.73125800	-0.66527400
N	3.70338200	-0.42469300	-0.40766400
C	-2.44582900	1.22540400	0.94512200
C	-1.20381400	0.39447700	0.81837900
C	-0.92627300	-0.32781300	-0.34485100
H	-1.65275700	-0.35150000	-1.15526400
C	0.28068100	-1.00371500	-0.47978800
H	0.50928800	-1.56871100	-1.38018200
C	1.19743000	-0.95765900	0.56897600
C	0.93982400	-0.23902600	1.73500000
H	1.67237400	-0.21993300	2.53830400
C	-0.26341700	0.44479800	1.84992900
H	-0.48174500	1.02717300	2.74161500
C	3.28215000	-0.07187800	-1.69234800
H	3.16805700	-0.89629400	-2.39329300
C	2.79156400	1.29401700	-2.02912500
H	3.59751300	2.04575800	-1.96291100
H	2.04171700	1.61249800	-1.28083500
C	2.17421400	1.32792900	-3.41912900
H	1.82080000	2.33163000	-3.67423000
H	1.31958100	0.64234000	-3.48205100
H	2.90200800	1.02290000	-4.18033800
H	6.19656800	1.90793100	1.93921500
C	4.24257000	0.62389000	0.47031200
H	4.27346700	0.22702500	1.49056000
H	3.57476200	1.50139200	0.47903400
C	5.64404900	1.02099400	0.03474900
H	5.63455500	1.29892000	-1.02864700
H	6.29706300	0.14242200	0.11883600
C	6.17205300	2.17182000	0.87442900
H	7.18826200	2.44997600	0.57775100
H	5.53875600	3.06197900	0.76824600
N	-3.64284200	0.62475100	0.70017500
C	-3.90738600	-0.80962300	0.76230700
H	-4.40609000	-1.03130300	1.71934000
H	-2.97132100	-1.37117400	0.73469400
C	-5.75679100	0.97465900	-0.44355900
N	-6.04990700	-0.44794300	-0.34926800
H	-6.70070800	1.53321000	-0.40848600
H	-5.26452600	1.21136600	-1.41244700

C	-4.81739300	-1.21874500	-0.37796700
H	-4.28465500	-1.07958100	-1.34556800
H	-5.06220600	-2.28461100	-0.28630200
C	-6.94791000	-0.86492500	-1.40762700
H	-7.18245700	-1.92999600	-1.30155900
H	-7.88441800	-0.29941500	-1.34748100
H	-6.51187600	-0.70523800	-2.41463800
C	-4.86135500	1.42635200	0.69313500
H	-4.58330400	2.47699000	0.58474200
H	-5.38441500	1.30433900	1.65454100

Clomipramine

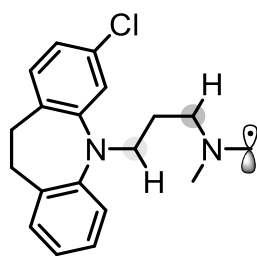


E = -847.555701

H_{Corr.} = 0.41038

C	0.30578900	3.15410200	-1.45399400
C	0.34096500	1.78125800	-1.25421300
C	-0.50978300	1.13778800	-0.33742600
C	-1.41645700	1.92658700	0.40578500
C	-1.43963800	3.30583700	0.16906700
C	-0.60037400	3.93255100	-0.74159600
H	0.98337300	3.60808500	-2.17360600
H	1.04738800	1.19240700	-1.83337100
H	-2.14338400	3.90593200	0.74694900
H	-0.64691500	5.00923200	-0.88408400
C	-2.37748200	1.43484400	1.46735000
H	-3.40697300	1.57463700	1.10046200
H	-2.28138300	2.10278000	2.33509900
C	-2.23381200	-0.00988400	1.93042500
H	-2.92832500	-0.18767800	2.76081500
H	-1.21581900	-0.17808300	2.31046400
N	-0.41620700	-0.27071200	-0.18647900
C	-1.60595100	-1.04745600	-0.24361300
C	-1.85202400	-1.91768400	-1.30884500
C	-2.52129400	-0.96023600	0.81378500
C	-3.00636100	-2.69572800	-1.32975600
H	-1.13985900	-1.97791000	-2.12977100
C	-3.68199200	-1.73195200	0.76924800
C	-3.92849400	-2.60096000	-0.29076800
H	-3.18816100	-3.36796900	-2.16518500
H	-4.39294600	-1.66033700	1.59201500
H	-4.83354700	-3.20354100	-0.30352500
C	0.81945100	-0.94299100	-0.57071600
H	0.64699600	-2.01789000	-0.43890400
H	1.06413700	-0.80850500	-1.64148800
C	1.99995500	-0.52990700	0.29713900
H	1.84452300	-0.90062400	1.32045300
H	2.04933200	0.56516800	0.35895300
C	3.29609000	-1.08925200	-0.26222000
H	3.15662600	-2.15553400	-0.49961600
H	3.52634900	-0.58099800	-1.22902900
N	4.42539700	-0.98905500	0.64836200
C	5.57758900	-1.67238900	0.09245500
H	5.91672100	-1.21656500	-0.86137700
H	6.41281600	-1.63732000	0.80086000
H	5.33570300	-2.72391100	-0.09992500
C	4.76027100	0.39096400	0.94771500
H	5.64095400	0.42223600	1.59846100
H	4.98936100	0.97236400	0.02949100
H	3.94002000	0.88943100	1.47375500

Clomipramine_{I1}

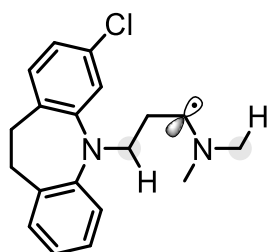


E = -846.899095

H_{Corr.} = 0.396916

C	2.93761500	-2.91313100	-0.96105100
C	1.76580500	-2.16815600	-0.94514300
C	1.63080200	-1.01406700	-0.15514900
C	2.72590100	-0.59919700	0.63448300
C	3.89787300	-1.36134400	0.58391700
C	4.02255600	-2.50685300	-0.19167200
H	3.00127000	-3.80094900	-1.58610700
H	0.93840200	-2.47975900	-1.57692000
H	4.73828800	-1.04009600	1.20025700
H	4.95046000	-3.07321200	-0.19097000
C	2.76223600	0.59860200	1.56050600
H	3.48656200	1.32549800	1.15922100
H	3.18266500	0.26462500	2.51972200
C	1.45264900	1.33618900	1.82088700
H	1.63237100	2.12215200	2.56493900
H	0.71342600	0.64256700	2.24708500
N	0.39607000	-0.31774300	-0.16551400
C	0.41183100	1.08195000	-0.42417000
C	-0.08281300	1.60726100	-1.61986300
C	0.91263600	1.93893200	0.56403400
C	-0.07627800	2.98155200	-1.83945100
H	-0.47388500	0.93646300	-2.38281800
C	0.93082400	3.31268400	0.32208800
C	0.43554500	3.83891900	-0.86830800
H	-0.46442400	3.38054900	-2.77377200
H	1.32581200	3.97761700	1.08974600
H	0.44562700	4.91324800	-1.03589000
C	-2.05865100	-0.43120600	0.09298200
H	-2.28491100	0.54460300	-0.35873900
H	-1.85943000	-0.25423000	1.16003600
N	-4.52429700	-0.73816700	0.23244100
C	-5.64920600	-1.31821700	-0.32655800
H	-6.61276800	-0.92790900	-0.01165600
H	-5.54359500	-1.73729000	-1.32345100
C	-4.64918800	-0.28070500	1.60201000
H	-5.63338700	0.17520700	1.74353100
H	-4.54425900	-1.11398800	2.31975300
H	-3.89078400	0.47446300	1.83033600
C	-0.81192000	-1.04528200	-0.52664300
H	-0.69901900	-2.06729900	-0.14046100
H	-0.94833000	-1.14198300	-1.62146300
C	-3.24989300	-1.35519200	-0.09777300
H	-3.10964700	-2.27908600	0.49927400
H	-3.30279000	-1.66625900	-1.15089500

Clomipramine I₂

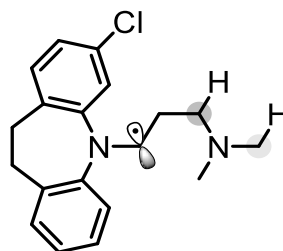


E = -846.901736

H_{Corr.} = 0.396947

C	2.83391500	-3.00592700	-0.94795500
C	1.69399200	-2.21313300	-0.94102300
C	1.59969600	-1.05531900	-0.15014300
C	2.70433200	-0.68762700	0.64971000
C	3.84409300	-1.49759700	0.60812400
C	3.92811200	-2.64626500	-0.16829500
H	2.86610600	-3.89479900	-1.57401500
H	0.85935100	-2.48886000	-1.57993500
H	4.69156000	-1.21243500	1.23256100
H	4.83170300	-3.25068800	-0.16054900
C	2.78236600	0.50528400	1.57955900
H	3.54090200	1.20183300	1.18765200
H	3.17871500	0.15117800	2.54187200
C	1.50263300	1.29685600	1.82915800
H	1.70796400	2.07324600	2.57667800
H	0.73084200	0.63400700	2.24638100
N	0.39608700	-0.30793300	-0.17176800
C	0.47460400	1.08992800	-0.42648900
C	0.01516900	1.63764800	-1.62648100
C	1.00121100	1.92374700	0.56809300
C	0.08337800	3.01043100	-1.84413300
H	-0.39696000	0.98471500	-2.39377000
C	1.08021300	3.29594500	0.32869800
C	0.62075200	3.84427000	-0.86606300
H	-0.27716500	3.42672600	-2.78199400
H	1.49504600	3.94248700	1.10164800
H	0.67872000	4.91742100	-1.03181000
C	-2.06146300	-0.32827900	0.08942300
H	-2.18530000	0.69884800	-0.30456100
H	-1.86228100	-0.20779800	1.16872900
C	-3.27746600	-1.14755000	-0.16842900
H	-3.27229900	-1.83496100	-1.01644000
N	-4.53902200	-0.66321500	0.16216000
C	-5.63708900	-1.58323700	-0.05436900
H	-5.66683800	-2.37831300	0.71237500
H	-6.58814100	-1.04031900	-0.02841300
H	-5.53657800	-2.05557000	-1.03697300
C	-4.66719200	0.09379500	1.39192600
H	-5.66513400	0.54181100	1.43923300
H	-4.52899900	-0.54493100	2.28429000
H	-3.93171800	0.90238600	1.42824800
C	-0.84003000	-0.98267600	-0.54125100
H	-0.77425800	-2.01233400	-0.16750200
H	-0.98205700	-1.05736900	-1.63682200

Clomipramine I₃



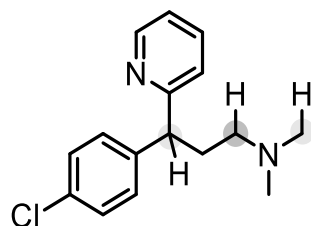
E = -846.903205

H_{Corr.} = 0.39659

C	-1.07313900	-2.59340400	-1.46771600
C	-0.77795500	-1.27988300	-1.14024400
C	0.27618400	-0.95737800	-0.26897700
C	1.06885700	-1.98943200	0.27086600
C	0.75523100	-3.30540500	-0.09096200
C	-0.29837200	-3.62350100	-0.93733000
H	-1.89613000	-2.80928200	-2.14538400
H	-1.35567700	-0.46279000	-1.56954300
H	1.36450800	-4.10647600	0.32858700
H	-0.51164000	-4.66145400	-1.18034000

C	2.23941100	-1.81984700	1.21413800
H	3.15331300	-2.14005600	0.68868700
H	2.11016600	-2.53351000	2.03999300
C	2.48838700	-0.43004300	1.79169200
H	3.31922400	-0.48923400	2.50545200
H	1.60307500	-0.09593800	2.35130100
N	0.48960000	0.41726500	0.02955100
C	1.79802800	0.95190400	-0.16206900
C	2.05297700	1.86407000	-1.18554900
C	2.81235500	0.56065100	0.71817200
C	3.33178200	2.39047400	-1.34227400
H	1.24653400	2.14774600	-1.85911700
C	4.09205500	1.08539300	0.53661700
C	4.35491200	1.99801200	-0.48210000
H	3.53005400	3.09904400	-2.14292300
H	4.88758100	0.78319200	1.21699100
H	5.35631300	2.40420100	-0.60287300
C	-0.57953700	1.30990600	0.10734100
H	-0.28709500	2.35720300	0.06821200
C	-1.85739300	0.93542000	0.77828000
H	-1.91456500	1.37933100	1.78791800
H	-1.89359200	-0.15121100	0.92227900
C	-3.07329400	1.40954400	-0.00976200
H	-3.02274900	2.50406800	-0.10650800
H	-3.02492400	1.00471700	-1.04718400
N	-4.34326800	1.07098400	0.61443100
C	-5.42802100	1.78933300	-0.02751100
H	-5.52669100	1.52770400	-1.10194900
H	-6.37796100	1.55436400	0.46593100
H	-5.26174000	2.86992000	0.04656300
C	-4.59913200	-0.35727500	0.56066600
H	-5.56809600	-0.57764100	1.02198900
H	-4.61919800	-0.73476100	-0.48418800
H	-3.83504500	-0.91810900	1.10856900

Chlorpheniramine



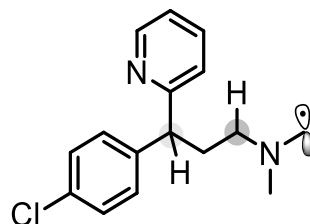
$E = -1190.486931$

$H_{\text{Corr.}} = 0.335658$

Cl	4.91669700	0.85026500	0.42593900
N	-2.25224400	1.39449100	0.94221500
N	-1.50404100	-3.69662900	-0.08002600
C	-1.76395300	1.29426400	-0.29883100
C	-1.91381300	2.31489500	-1.24269900
C	-2.59440800	3.47100600	-0.88727400
C	-3.10632800	3.57671000	0.40270400
C	-2.90580900	2.51211400	1.27368100
C	-0.98628000	0.04650800	-0.66348800
C	-1.52967500	-1.21036600	0.01912700
C	-0.82023900	-2.46706600	-0.45580300
C	-0.84727100	-4.83620200	-0.69155000
C	-1.55525100	-3.86763000	1.36061100
C	0.49079400	0.25840600	-0.39084700
C	1.42084700	0.20544500	-1.42937900
C	2.78173300	0.38524400	-1.19151200
C	3.20752300	0.62289700	0.10817700
C	2.30453200	0.68619600	1.16471000
C	0.95092400	0.50456100	0.90675100
H	-1.49502000	2.19361300	-2.24037700
H	-2.72599800	4.27702200	-1.60521600
H	-3.64820000	4.46006700	0.72834700
H	-3.29124500	2.55734800	2.29239800
H	-1.09320800	-0.08871500	-1.75171800
H	-2.60370600	-1.29985800	-0.19954800

H	-1.44163300	-1.09120900	1.10640300
H	-0.75317600	-2.45000500	-1.55555800
H	0.22834700	-2.47552300	-0.07938200
H	-1.38757200	-5.75736800	-0.44585800
H	0.20206300	-4.95107000	-0.34780900
H	-0.83758400	-4.72526600	-1.78197900
H	-2.03222300	-4.82440100	1.60002600
H	-0.54240000	-3.86365200	1.81632000
H	-2.14593700	-3.07458200	1.82985400
H	1.07888400	0.01368400	-2.44614300
H	3.50186200	0.33951500	-2.00408800
H	2.65930600	0.87702400	2.17407900
H	0.23763200	0.56194900	1.72768300

Chlorpheniramine_I

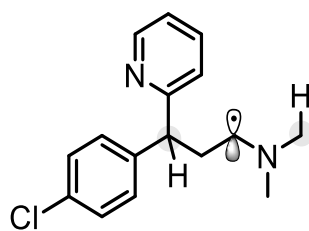


$E = -1189.829371$

$H_{\text{Corr.}} = 0.322277$

Cl	4.98877700	0.34063300	0.43063400
N	-2.10821900	1.59379300	0.93030900
N	-1.83386300	-3.55643800	0.02011700
C	-1.61289900	1.43148900	-0.30096900
C	-1.63621800	2.45352200	-1.25470800
C	-2.19422500	3.67900800	-0.91912500
C	-2.71291700	3.85043600	0.36106400
C	-2.64313800	2.77811400	1.24283600
C	-0.96606000	0.10483300	-0.64318700
C	-1.63350600	-1.07615700	0.06414000
C	-1.04179100	-2.40233600	-0.38014500
C	-1.45085200	-4.77836300	-0.65719600
C	-2.17493600	-3.68578300	1.35418100
C	0.52540900	0.17229300	-0.37450600
C	1.44338900	0.01728300	-1.41352900
C	2.81577600	0.06680000	-1.17907400
C	3.26527000	0.27642700	0.11746500
C	2.37497000	0.43891300	1.17422500
C	1.00966100	0.38716600	0.91984200
H	-1.21619000	2.27907600	-2.24398600
H	-2.22651900	4.48815400	-1.64482100
H	-3.16168900	4.78983600	0.67100100
H	-3.03867700	2.87310500	2.25414700
H	-1.08848800	-0.03881400	-1.72875400
H	-2.70991200	-1.06443700	-0.15941600
H	-1.53744600	-0.94443300	1.14875900
H	-0.97624300	-2.42164300	-1.47912600
H	-0.00524700	-2.50497500	0.00031600
H	-2.15333100	-5.57768800	-0.40081400
H	-0.43484100	-5.10439900	-0.37237900
H	-1.47695500	-4.62833400	-1.74202800
H	-2.65953500	-4.61487400	1.64094000
H	-2.40188700	-2.78336600	1.91191200
H	1.08216400	-0.15113400	-2.42781100
H	3.52641700	-0.05740900	-1.99176700
H	2.74875800	0.60479500	2.18107600
H	0.30738300	0.52242200	1.74110100

Chlorpheniramine_I

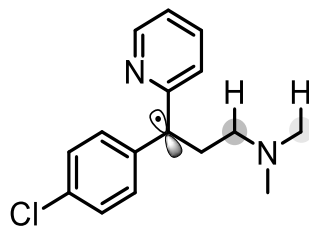


E = -1189.832756

H_{Corr.} = 0.322231

Cl	4.70144800	1.53217100	0.46742200
N	-2.47415700	1.00438300	0.92223600
N	-0.74091000	-3.86772600	-0.13152900
C	-1.94657500	1.00524200	-0.30668600
C	-2.19770500	2.03009400	-1.22404400
C	-3.02320100	3.08268400	-0.85433800
C	-3.57579100	3.08309600	0.42319500
C	-3.26803900	2.02235400	1.26754200
C	-1.00979400	-0.12315300	-0.68425600
C	-1.38503000	-1.45218400	-0.02780300
C	-0.52919000	-2.55550400	-0.53829800
C	0.23257100	-4.83273900	-0.60186200
C	0.42369800	0.27664300	-0.39262000
C	1.33844200	0.45217300	-1.43131700
C	2.65395800	0.83537400	-1.18039300
C	3.04911300	1.04763900	0.13316300
C	2.15936900	0.88779400	1.19072300
C	0.85114600	0.50540300	0.91925500
H	-1.74312800	1.99275600	-2.21275200
H	-3.23478900	3.88970600	-1.55177900
H	-4.22941600	3.88295300	0.75936800
H	-3.68184200	1.98659600	2.27549600
H	-1.08916500	-0.25370100	-1.77534700
H	-2.46142800	-1.64142000	-0.21585400
H	-1.30401800	-1.34125900	1.06443400
H	-0.08782300	-2.46210600	-1.53267800
H	-0.16065900	-5.84791400	-0.48014300
H	1.18695600	-4.75778900	-0.05062600
H	0.43517100	-4.66627200	-1.66485500
H	1.02091000	0.28070100	-2.45961900
H	3.36302200	0.96581400	-1.99352900
H	2.48873400	1.06368100	2.21135900
H	0.14726900	0.39010000	1.74216200
C	-1.15192600	-4.09619500	1.23981100
H	-0.34456900	-3.85774400	1.95697800
H	-2.02732700	-3.49031900	1.48981500
H	-1.42332300	-5.14960900	1.36403300

Chlorpheniramine I₃



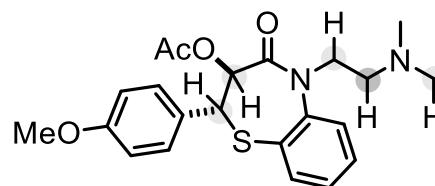
E = -1189.848604

H_{Corr.} = 0.322582

Cl	5.20392800	0.39919700	-0.31077400
N	-2.90167100	1.11695200	-0.15088100
N	-1.92368000	-3.35645000	-0.05488100
C	-1.62274900	1.38318800	0.21333600
C	-1.19641200	2.71131700	0.43159500
C	-2.08502300	3.75606300	0.23662700
C	-3.38484100	3.47358800	-0.17516300

C	-3.73428100	2.13351400	-0.34327700
C	-0.75843500	0.23883900	0.43289600
C	-1.40089000	-1.06892800	0.78537300
C	-2.20294200	-4.11041300	-1.26325100
C	0.67657100	0.30341800	0.27123400
C	1.29949100	1.25985100	-0.56710100
C	2.67237300	1.29263200	-0.74880200
C	3.47011900	0.35911700	-0.09208300
C	2.90204600	-0.61560800	0.72345300
C	1.52690000	-0.64452000	0.89014500
H	-0.19058800	2.90947200	0.79145100
H	-1.76992100	4.78107400	0.41716700
H	-4.11438800	4.26029100	-0.34396900
H	-4.74847700	1.87025500	-0.64630900
H	-2.44121000	-0.90607300	1.08217500
H	-0.88894300	-1.51098200	1.65115700
H	-2.63711700	-5.08310600	-1.00562400
H	-1.28825600	-4.29217300	-1.86527600
H	-2.92150200	-3.56886900	-1.88820100
H	0.68768700	1.96558800	-1.12282100
H	3.12507400	2.02750700	-1.40920100
H	3.53480100	-1.34418800	1.22325200
H	1.10581700	-1.41304100	1.53355500
C	-1.01961600	-4.10755700	0.79631700
H	-0.03061600	-4.26413300	0.31530500
H	-0.85774600	-3.59626600	1.75131600
H	-1.44998600	-5.09022900	1.01857100
C	-1.38440600	-2.04741700	-0.39000500
H	-0.35171500	-2.14154800	-0.79481100
H	-1.99968200	-1.61595000	-1.19199600

Diltiazem



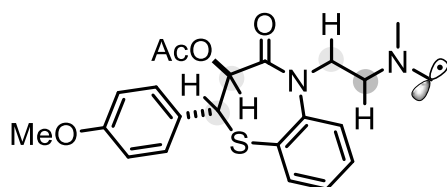
E = -1662.116187

H_{Corr.} = 0.477624

S	-0.37874800	2.24774700	-1.15310200
C	0.60555600	-0.36064500	0.18774500
N	1.72985700	0.07199300	-0.46524700
C	1.32365100	2.49460100	-0.68424000
C	2.19066800	1.41314500	-0.43672700
C	-2.41261400	0.85560400	0.02725600
C	-4.87071500	-0.37364800	-0.55656000
O	-6.09902900	-0.90964700	-0.76642400
O	-0.76001700	-0.01541100	2.14976700
C	0.02956800	-0.65790100	3.03672200
O	1.23877800	-0.62539200	2.98027400
O	0.18704900	-1.50408400	0.08069300
N	3.73258200	-3.02377400	-1.16281100
C	-6.23310600	-1.89193200	-1.77409000
H	-7.28310800	-2.18837600	-1.77524700
H	-5.97024900	-1.48999300	-2.76157000
H	-5.60973100	-2.77044600	-1.56121600
C	-1.11744900	1.53260000	0.38807900
H	-1.34383500	2.36275300	1.07009400
C	-0.07953900	0.65708700	1.09818300
H	0.68666600	1.30505200	1.54213900
C	-0.78562000	-1.39683200	4.04409700
H	-0.14579900	-1.74141900	4.85710400
H	-1.59124300	-0.76599300	4.42912600
H	-1.24995500	-2.26035400	3.55592400
C	2.45479000	-0.92655100	-1.26121900
H	3.07458000	-0.39400700	-1.98932300
H	1.70912500	-1.50308400	-1.81931000

C	3.30788400	-1.85612600	-0.40578800
H	2.74966300	-2.14319300	0.50858000
H	4.20667000	-1.32041400	-0.07058800
C	4.90994400	-3.63032900	-0.56873000
H	5.22307700	-4.49457600	-1.16542600
H	5.73726000	-2.91224100	-0.54705900
H	4.72496100	-3.97995100	0.46756800
C	2.66665300	-4.00870200	-1.25778400
H	2.39659700	-4.41805000	-0.26331900
H	1.76276900	-3.57071900	-1.69260900
H	2.98450300	-4.83815700	-1.89921100
C	-3.57323900	1.19285500	0.73357600
H	-3.51927200	1.94083300	1.52373100
C	-4.78838800	0.59047400	0.45256800
H	-5.69012900	0.85257000	1.00028300
C	-3.72582000	-0.72032900	-1.27655200
H	-3.76158300	-1.46384000	-2.06682500
C	-2.51274600	-0.10351700	-0.97996200
H	-1.63113100	-0.38581100	-1.55134500
C	3.54072400	1.66675900	-0.18434700
H	4.20628000	0.83383300	0.02874600
C	4.03448500	2.96578900	-0.19360600
H	5.08952900	3.13900200	0.00184800
C	3.17838300	4.03717900	-0.43289400
H	3.55688500	5.05588400	-0.43219900
C	1.82871300	3.79741000	-0.66421200
H	1.14542100	4.62353800	-0.84741900

Diltiazem_{I1}



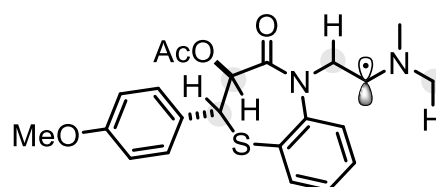
E = -1661.458101

H_{Corr.} = 0.46394

S	-0.36115200	2.17643700	-1.20088400
C	0.59260200	-0.39221100	0.21870800
N	1.73598500	0.02293400	-0.41438800
C	1.33176000	2.43797700	-0.70560100
C	2.19487500	1.36501800	-0.41149600
C	-2.42438900	0.83393700	-0.01335700
C	-4.88487300	-0.38997500	-0.59763400
O	-6.11474600	-0.92112900	-0.80994200
O	-0.80753600	-0.00484200	2.14714300
C	-0.03350600	-0.63673700	3.05551800
O	1.17658300	-0.61092000	3.01426200
O	0.17331400	-1.53607400	0.12485400
N	3.80117800	-3.05054400	-0.99506600
C	-6.24195800	-1.93585200	-1.78599900
H	-7.29441200	-2.22332800	-1.79367400
H	-5.96029300	-1.56978500	-2.78219200
H	-5.62976600	-2.81174200	-1.53373200
C	-1.12874000	1.50942500	0.34780300
H	-1.35769100	2.35970300	1.00360300
C	-0.10752600	0.64535300	1.09468900
H	0.65271100	1.30003100	1.53916600
C	-0.86535300	-1.35614900	4.06305100
H	-0.24074600	-1.67721000	4.89725300
H	-1.68367100	-0.72265300	4.41528300
H	-1.31220000	-2.23492700	3.58576800
C	2.48434700	-0.99568600	-1.15832400
H	3.13560100	-0.48488700	-1.87493200
H	1.76375800	-1.59427400	-1.72730700
C	3.29497500	-1.91427700	-0.24718600
H	2.66618300	-2.24540600	0.59576600
H	4.14651100	-1.37037700	0.18033300
C	5.19337200	-3.39903500	-0.80120800
H	5.49141600	-4.13619500	-1.55421900

H	5.82423500	-2.51221300	-0.92257900
H	5.37927600	-3.83271400	0.19596300
C	2.91635400	-4.08405700	-1.23954400
H	1.85455400	-3.86202300	-1.19006300
H	3.27419400	-4.91819200	-1.83561600
C	-3.59244700	1.20383600	0.66374800
H	-3.54350500	1.97536600	1.43125200
C	-4.80891400	0.60449900	0.38212400
H	-5.71645800	0.89189400	0.90708700
C	-3.73242000	-0.76927100	-1.28856600
H	-3.76308900	-1.53674900	-2.05579900
C	-2.51816700	-0.15466800	-0.99225600
H	-1.63096500	-0.46231200	-1.54124800
C	3.53946700	1.62752900	-0.13961200
H	4.20243800	0.80250300	0.10911900
C	4.03224400	2.92647700	-0.17458400
H	5.08305500	3.10646800	0.03689100
C	3.18007000	3.98961400	-0.45997200
H	3.55752600	5.00848700	-0.47993000
C	1.83547000	3.74146900	-0.71124500
H	1.15525200	4.56123900	-0.93076500

Diltiazem_{I2}



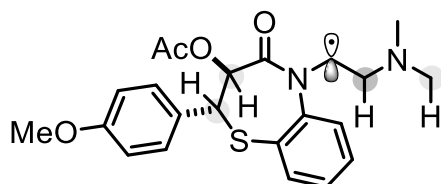
E = -1661.460231

H_{Corr.} = 0.463992

S	-0.39002000	2.37688100	-0.91357500
C	0.63867300	-0.38440300	0.03212300
N	1.73947100	0.12868400	-0.60646300
C	1.33398000	2.55721300	-0.49486600
C	2.20788600	1.45376900	-0.44073200
C	-2.38445200	0.85082400	0.16349800
C	-4.87860100	-0.27602700	-0.47185200
O	-6.12155700	-0.76955200	-0.70046300
O	-0.64420000	-0.29641900	2.07458700
C	0.18220000	-1.04187300	2.83937600
O	1.38822400	-0.98775400	2.74632000
O	0.21796300	-1.50908700	-0.19093700
N	3.73179300	-2.98151800	-1.05711100
C	-6.30177100	-1.63298100	-1.80495600
H	-7.35637700	-1.91268500	-1.80643300
H	-6.06061200	-1.12864600	-2.75014400
H	-5.68794200	-2.53835500	-1.70891200
C	-1.06916300	1.47072100	0.55157800
H	-1.25873900	2.20551500	1.34510100
C	-0.00716200	0.50977500	1.09166500
H	0.78112300	1.09428700	1.58307500
C	-0.59072000	-1.91891000	3.76622100
H	0.07960200	-2.35765400	4.50602300
H	-1.39030000	-1.35704400	4.25626700
H	-1.06092400	-2.71784200	3.18295500
C	2.51197700	-0.81050400	-1.43784700
H	3.13020200	-0.18869500	-2.10884000
H	1.79664300	-1.34300600	-2.07735600
C	3.28277900	-1.75608000	-0.58920300
H	3.76299800	-1.38800700	0.31639800
C	4.24069600	-3.87455700	-0.03255900
H	4.81303800	-4.68454000	-0.49679300
H	4.90541600	-3.32396800	0.64069600
H	3.42534200	-4.31438500	0.56810900
C	-3.51771400	1.12418800	0.93832100
H	-3.42810800	1.78168600	1.80222000
C	-4.75062300	0.57183000	0.63221300
H	-5.63128300	0.78495200	1.23293200

C	-3.76126100	-0.55808000	-1.26018700
H	-3.83270100	-1.21141200	-2.12428600
C	-2.53000200	0.00736300	-0.93751000
H	-1.67105800	-0.22243400	-1.56404800
C	3.57458500	1.67774100	-0.25071500
H	4.25064900	0.82644600	-0.20253800
C	4.07244000	2.96829200	-0.12095300
H	5.13946900	3.11737300	0.02314800
C	3.20895100	4.05996400	-0.15905800
H	3.59237800	5.07084500	-0.04896000
C	1.84683800	3.84782900	-0.33614600
H	1.15779500	4.68869900	-0.37073300
C	2.94473100	-3.66140800	-2.06924500
H	1.94375100	-3.94041500	-1.69387900
H	2.82283900	-3.03468400	-2.95795700
H	3.46923100	-4.57189700	-2.37489500

Diltiazem I₃



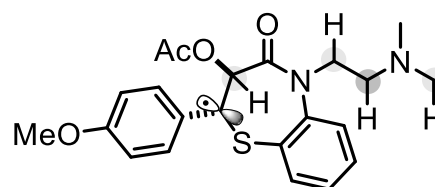
E = -1661.456198

H_{Corr.} = 0.463404

S	-0.21693100	2.11630300	-1.28711400
C	0.70361700	-0.35960300	0.22279200
N	1.90639800	0.02557200	-0.35514800
C	1.46516200	2.42430800	-0.78253500
C	2.33309300	1.38260800	-0.40655800
C	-2.31762800	0.92312100	-0.01312700
C	-4.83308900	-0.22261800	-0.51577400
O	-6.08620800	-0.71096000	-0.69197700
O	-0.71013900	0.07272000	2.13285000
C	0.04478400	-0.58013300	3.04206300
O	1.25466500	-0.60369200	2.99054500
O	0.25302200	-1.48496700	0.10156400
N	3.45211900	-3.24544800	-1.14907600
C	-6.26433700	-1.76970700	-1.61173000
H	-7.32834100	-2.01072000	-1.59924900
H	-5.97373300	-1.46983800	-2.62728900
H	-5.68911000	-2.65698600	-1.31591200
C	-0.99279100	1.56359300	0.30194000
H	-1.18138100	2.45570100	0.91340400
C	0.00872000	0.69902900	1.07728200
H	0.77093900	1.35160200	1.52125900
C	-0.80713700	-1.25402300	4.06432200
H	-0.18552000	-1.61298200	4.88516000
H	-1.57858900	-0.57376800	4.43493300
H	-1.31639800	-2.10273700	3.59552000
C	2.74526100	-0.93382800	-0.93818100
C	3.31650400	-0.59559300	-1.80109500
C	4.13834600	-4.33165700	-0.47699800
H	4.37093800	-5.12508100	-1.19612300
H	5.07983600	-3.97515900	-0.04339900
H	3.52803600	-4.77507400	0.33661300
C	-3.46387100	1.38210800	0.64664500
H	-3.37646600	2.19372100	1.36800200
C	-4.70725700	0.82172000	0.40515100
H	-5.59780700	1.17832000	0.91658300
C	-3.70292300	-0.69077200	-1.18884000
H	-3.77239000	-1.49838600	-1.91108900
C	-2.46069600	-0.11472900	-0.93358800
H	-1.59132300	-0.49294100	-1.46630600
C	3.66508200	1.67048000	-0.10010400
H	4.31869700	0.85730500	0.20984900
C	4.14419400	2.97160100	-0.18208800
H	5.18368100	3.17721600	0.05953600
C	3.29090200	4.00661500	-0.55806500

H	3.65841800	5.02740500	-0.62083300
C	1.95831300	3.73044800	-0.84318200
H	1.27895800	4.52999000	-1.12979100
C	2.23283900	-3.72775600	-1.77631800
H	1.53555400	-4.17468000	-1.03963800
H	1.71142600	-2.90026600	-2.27068500
H	2.48000700	-4.48605500	-2.52785900
C	3.16964600	-2.16209000	-0.21794300
H	2.42111900	-2.45259800	0.54549300
H	4.10610700	-1.94719600	0.33147800

Diltiazem I₄



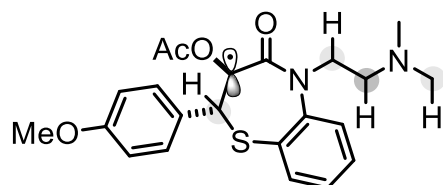
E = -1661.473032

H_{Corr.} = 0.464654

S	-0.68492400	2.23774000	-0.70704200
C	0.81828300	-0.52298000	0.08639800
N	1.78523700	0.23651400	-0.52082700
C	0.99148700	2.56159400	-0.20012000
C	2.02415200	1.60277400	-0.21829900
C	-2.49402500	0.31143900	0.00449800
C	-5.08083100	-0.70266400	-0.56798900
O	-6.28431000	-1.28285900	-0.80148400
O	-0.60519700	-0.66884700	2.03914600
C	0.32646900	-1.20066200	2.86065300
O	1.49838500	-0.90247800	2.79897300
O	0.64950400	-1.70563700	-0.16537600
N	4.30529100	-2.28984100	-1.68617900
C	-7.30372800	-0.48944800	-1.37461600
H	-8.17436600	-1.13818300	-1.48156000
H	-7.56228900	0.35818600	-0.72600700
H	-7.00902600	-0.11395800	-2.36364200
C	-1.19167400	0.84641800	0.25958000
C	-0.09704000	0.22271400	1.06025500
H	0.47763300	1.00191500	1.58038700
C	-0.28865700	-2.18067100	3.80163900
H	0.44124400	-2.48027700	4.55417600
H	-1.17640700	-1.75401200	4.27647600
H	-0.61106600	-3.06101300	3.23496600
C	5.60520800	-2.73960600	-1.22262000
H	6.03307800	-3.44369200	-1.94521000
H	6.28986000	-1.88939400	-1.12763000
H	5.54729500	-3.25164500	-0.24039700
C	-2.83853700	-1.04098400	0.27368800
H	-2.09212800	-1.71304400	0.68293300
C	-4.09729800	-1.52881900	-0.00619700
H	-4.34604700	-2.56890900	0.19125000
C	-4.77326000	0.63029000	-0.85006000
H	-5.51185300	1.30010900	-1.28037100
C	-3.50454300	1.11885300	-0.56806300
H	-3.30332100	2.16833100	-0.77538000
C	3.32987600	2.01921200	0.05292800
H	4.12730000	1.28144900	0.06651500
C	3.62137400	3.35244000	0.31390400
H	4.64794400	3.64593000	0.51635700
C	2.60007500	4.29698900	0.33829900
H	2.81550400	5.33949600	0.55601500
C	1.29266600	3.89492000	0.09647800
H	0.48175100	4.61919400	0.12451000
C	3.43037000	-3.43463400	-1.88487100
H	3.29326900	-4.01339500	-0.94920300
H	2.44005500	-3.12011700	-2.22823400
H	3.85770600	-4.09899100	-2.64406000
C	3.72383300	-1.32888200	-0.76161600
H	3.27732100	-1.82751400	0.12305500

H	4.53422000	-0.68958700	-0.38615800
C	2.67232700	-0.46907900	-1.45657500
H	3.14511800	0.27822900	-2.10139700
H	2.03608400	-1.09638200	-2.08952300

Diltiazem_I₅



E = -1661.460941

H_{Corr.} = 0.464167

S	-0.65429100	1.96095700	-1.20208700
C	0.74340800	-0.55110600	0.02577700
N	1.75680000	0.14855100	-0.56697900
C	0.95192700	2.47897600	-0.63059000
C	1.96333900	1.53885200	-0.36668000
C	-2.60974200	0.57442500	0.08833400
C	-5.14742900	-0.46140000	-0.49008000
O	-6.41560700	-0.87449100	-0.73568300
O	-0.59965000	-0.39205500	2.03777900
C	0.39887200	-0.82864200	2.87019900
O	1.56305900	-0.59982400	2.65807000
O	0.63720400	-1.77218900	-0.08272400
N	4.39415800	-2.41858000	-1.31064300
C	-6.60441400	-2.18280900	-1.23707000
H	-7.68037900	-2.30897800	-1.36612800
H	-6.10614400	-2.31488200	-2.20657400
H	-6.23402100	-2.93833000	-0.53158100
C	-0.23901400	0.19641400	0.85350600
C	-0.17404000	-1.59291700	4.01222500
H	0.59505700	-1.75786200	4.76719100
H	-1.02839200	-1.06275800	4.44158300
H	-0.53790000	-2.55923200	3.64666900
C	5.66330500	-2.79184700	-0.71335300
H	6.15426600	-3.55313300	-1.33016800
H	6.32584500	-1.92113900	-0.65362900
H	5.54128900	-3.20689300	0.30816400
C	-3.75808000	1.34923000	0.28432500
H	-3.66085700	2.36571000	0.66480000
C	-5.01502100	0.84251200	0.00014400
H	-5.91298200	1.43612000	0.15221800
C	-4.01044400	-1.24661500	-0.69193100
H	-4.08738800	-2.26233700	-1.06753200
C	-2.75253900	-0.72063200	-0.40480600
H	-1.86987200	-1.34264000	-0.55713500
C	3.21376500	1.98902400	0.06211900
H	3.98794300	1.26315800	0.29650100
C	3.46998000	3.34780000	0.20310900
H	4.45145300	3.67565200	0.53585400
C	2.47099800	4.27990000	-0.06407700
H	2.66476000	5.34318800	0.05010300
C	1.21453700	3.84096400	-0.46602400
H	0.41808300	4.55403100	-0.66688700
C	3.55495000	-3.59716800	-1.45715200
H	3.35411800	-4.08212800	-0.48038100
H	2.58981700	-3.34171200	-1.90519000
H	4.04999900	-4.32459400	-2.11009400
C	3.73236700	-1.38728600	-0.52512600
H	3.23662800	-1.80932000	0.37241800
H	4.50378700	-0.69380300	-0.16426300
C	2.71423200	-0.62310400	-1.36701600
H	3.21868900	0.06983600	-2.04821400
H	2.13339400	-1.32323100	-1.97692200
C	-1.25062300	1.16981800	0.36051600
H	-1.35729000	1.97228600	1.10831000

H radical



E = -0.499958

H_{Corr.} = 0.00236

H	0.00000000	0.00000000	0.00000000
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TMS

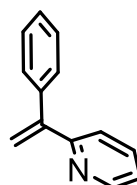


C_{NMR} isotropic shielding tensor (ppm) =

176.72

Si	-0.00000200	-0.00004500	0.00002400
C	-0.39869400	-1.83600700	-0.10979800
H	0.39806500	-2.38209700	-0.63007200
H	-0.51043800	-2.27567600	0.88914700
H	-1.33433500	-2.00419300	-0.65752800
C	-1.39290500	0.89181200	0.89806400
H	-1.52144600	0.49968000	1.91464000
H	-1.18697700	1.96661500	0.97601500
H	-2.34561800	0.76977500	0.36780000
C	1.60951700	0.23697800	0.94620200
H	2.44067500	-0.27403900	0.44443600
H	1.86744200	1.30043800	1.02516200
H	1.53204700	-0.16646900	1.96351200
C	0.18206600	0.70725800	-1.73445200
H	-0.74337100	0.58243900	-2.31039000
H	0.41497000	1.77886400	-1.70082500
H	0.98911800	0.20504800	-2.28232900

1-Phenyl-1-pyridineethane



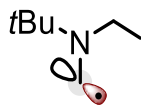
E = -556.458702

G_{Corr.} = 0.16307

C	0.04200400	-2.20243800	1.02110200
H	0.97033400	-2.71621700	1.25982400
H	-0.88418400	-2.71231900	1.27557800
C	0.03128900	-0.97497600	0.47869300
C	1.31842200	-0.30225700	0.15208500
C	2.38642100	-1.04602700	-0.36897900
C	3.58718200	-0.40591700	-0.64150000
H	2.26307200	-2.10532500	-0.57740700
C	2.57644500	1.61923700	0.10213700
C	3.69425700	0.95920700	-0.39701900
H	4.42555200	-0.96464900	-1.05061500
H	2.61495800	2.69112500	0.29733800
H	4.61269300	1.50319300	-0.59789800
C	-1.26460700	-0.31399300	0.16956200
C	-2.22776900	-1.02967900	-0.55420500
C	-1.58010300	0.98131300	0.60074600
C	-3.47226100	-0.47445400	-0.83583500
H	-1.98667300	-2.02923500	-0.91211300
C	-2.82736600	1.53311200	0.32269500
H	-0.84178700	1.54881300	1.15817600
C	-3.77727100	0.81125000	-0.39665100

H	-4.20165300	-1.04620200	-1.40523500
H	-3.05854500	2.53625100	0.67429400
H	-4.74848700	1.24922600	-0.61510100
N	1.41640800	1.01701100	0.36802500

³⁰I₁

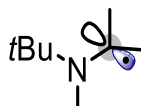


E = -370.207851

G_{Corr.} = 0.209085

N	0.14983000	-0.27351500	-0.41323000
C	0.33899800	-1.48800400	-1.04803600
H	-0.44776500	-1.86292600	-1.69231700
H	1.36065900	-1.73609000	-1.31960900
C	1.32943500	0.32865400	0.22641900
C	2.21411800	1.00377900	-0.81469600
C	2.12835700	-0.65041200	1.08364400
H	0.95687500	1.10968900	0.89977100
H	1.65330300	1.76681500	-1.36696000
H	3.07813300	1.48219900	-0.33760500
H	2.59273600	0.27128800	-1.53887900
H	1.48124900	-1.18319400	1.78938400
H	2.64801400	-1.39738200	0.47228300
H	2.88864500	-0.10453100	1.65497500
C	-1.18787700	0.12613500	0.08653100
C	-1.36492000	1.63675900	-0.08581400
C	-1.34891700	-0.27049100	1.55775100
H	-1.28111000	1.91059900	-1.14491000
H	-2.35823100	1.93635900	0.27042600
H	-0.62979300	2.22218200	0.47729600
H	-1.19930300	-1.35166200	1.67420500
H	-0.63343500	0.25056300	2.20564200
H	-2.35733900	-0.02173600	1.91253900
C	-2.28656300	-0.55658000	-0.72266000
H	-2.18158300	-0.34875000	-1.79455400
H	-2.29817900	-1.64151200	-0.57104600
H	-3.25747200	-0.16635100	-0.39687300

³⁰I₂



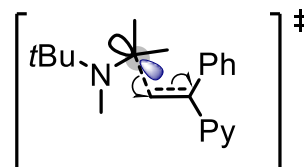
E = -370.206395

G_{Corr.} = 0.207465

N	0.12997800	-0.33329100	-0.54649800
C	0.11704600	-1.76417400	-0.81489800
H	-0.66054300	-2.01096300	-1.54521300
H	1.07508100	-2.05156400	-1.25860600
H	-0.04403700	-2.39859300	0.07586200
C	1.35799400	0.15116300	-0.03171200
C	2.24997800	-0.71821100	0.79187200
C	1.97268200	1.38078800	-0.61488900
H	2.95825800	-1.30928600	0.18105000
H	2.87006400	-0.10052400	1.45679500
H	1.69305600	-1.42798200	1.41544200
H	1.29437300	1.88602700	-1.30788800
H	2.28115000	2.10298200	0.15796400
H	2.89146900	1.12957200	-1.17628200
C	-1.10980200	0.19412600	0.10395100
C	-1.19149000	-0.24366900	1.56954300
C	-2.33909600	-0.30268500	-0.65285200
H	-0.34042100	0.15646100	2.13673400
H	-2.11382300	0.13047600	2.03239000

H	-1.19175700	-1.33656400	1.66951100
H	-2.24720000	-0.08704600	-1.72519500
H	-2.50746100	-1.37804200	-0.52497600
H	-3.23158400	0.21134500	-0.27624900
C	-1.10553300	1.71866300	0.04851600
H	-0.25915600	2.14351400	0.60051800
H	-1.06221500	2.07380400	-0.98867400
H	-2.02578100	2.10341400	0.50512100

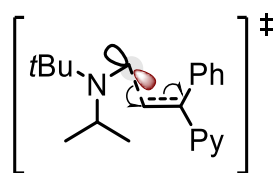
³⁰TS I₁-II₁



E = -926.672465

G_{Corr.} = 0.393274

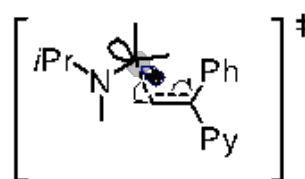
C	-3.16181100	0.78631300	-2.01605900
C	-3.06681300	0.75559600	-0.48673000
H	-3.86136100	0.02476400	-2.38174200
H	-3.51872500	1.76727300	-2.35395400
H	-2.18711700	0.60662700	-2.48394600
C	-2.10232400	1.84059500	-0.00297100
H	-2.06045100	1.85567000	1.09376700
H	-1.08087800	1.70152000	-0.37617100
H	-2.44747800	2.82356900	-0.34645300
N	-2.57084700	-0.57379900	-0.02801400
C	-3.47474000	-1.62265400	0.47013300
C	-2.81364200	-2.45551300	1.56179200
C	-4.00851700	-2.50590200	-0.65469700
H	-4.32210300	-1.11429800	0.94020400
H	-2.38912600	-1.81352200	2.34190100
H	-3.56072700	-3.11206300	2.02199700
H	-2.01352300	-3.09717800	1.17156600
H	-4.58465900	-1.92530300	-1.38449200
H	-3.18284400	-2.99544000	-1.18757600
H	-4.66285400	-3.28906000	-0.25293900
C	-1.30340000	-0.95054100	-0.38109400
H	-1.09321900	-2.01475500	-0.45145200
H	-0.74177600	-0.30739000	-1.05216700
C	0.36836500	-0.58234800	1.37615000
H	-0.36586600	0.10203700	1.79263400
H	0.29730300	-1.61422000	1.71242000
C	1.48326000	-0.10754300	0.73916200
C	-4.44198000	1.06600400	0.09507000
H	-4.72519400	2.07884900	-0.21291200
H	-5.22198100	0.38717300	-0.26998500
H	-4.43379600	1.04384600	1.19191000
C	1.58257200	1.34130200	0.46181400
C	1.27882400	2.28274400	1.45409800
C	1.89284600	1.81544800	-0.82202400
C	1.26635000	3.64611200	1.17373000
H	1.05757800	1.93555700	2.46243500
C	1.87507500	3.17618500	-1.10658000
H	2.13586500	1.10222100	-1.60752600
C	1.55915700	4.09994400	-0.11033900
H	1.03253800	4.35693800	1.96367700
H	2.10704300	3.51860400	-2.11294500
H	1.54919100	5.16462300	-0.33235400
C	2.50846700	-1.02056800	0.22446600
C	2.24252200	-2.38954300	0.02094900
C	4.68807800	-1.32430000	-0.46586300
C	3.25452900	-3.22490100	-0.42200100
H	1.24515400	-2.78584500	0.19472700
C	4.51700400	-2.69059300	-0.67133300
H	5.65748100	-0.86208100	-0.65860100
H	3.05821800	-4.28267400	-0.58346200
H	5.33979900	-3.30659600	-1.02276200
N	3.72950100	-0.50675300	-0.03510600

³⁰TS I₂-II₂

E = -926.669875

G_{Corr.} = 0.397047

N	-2.64373400	-0.28090900	0.61867800
C	-3.62222000	-0.64023000	-0.45972900
C	-3.68374600	0.47763500	-1.51338200
C	-4.99893600	-0.82705000	0.18365700
H	-2.70139300	0.65158600	-1.96946100
H	-4.37711700	0.18275900	-2.30984700
H	-4.04258200	1.42952800	-1.11076500
H	-4.97142800	-1.65275400	0.90527300
H	-5.34262400	0.07167500	0.70794000
H	-5.74517400	-1.06505500	-0.58489000
C	-1.45031200	-0.93861200	0.90543900
C	-0.00741000	-0.55873600	-0.94852200
H	-0.00900800	-1.59682100	-1.27644000
H	-0.81327900	0.07675700	-1.29745200
C	1.17949300	0.03800200	-0.57979200
C	-2.77440000	1.09309200	1.08834000
H	-2.13166600	1.79305500	0.52762200
H	-3.80894200	1.42508400	0.98729900
H	-2.52772600	1.16673200	2.14985000
C	-1.45051000	-2.44566600	1.02024100
H	-1.33636700	-2.98626200	0.07613500
H	-0.62170900	-2.75628500	1.66607600
H	-2.37976700	-2.79945300	1.49221100
C	-0.57717500	-0.28614200	1.93860200
H	-1.03059900	-0.35703600	2.94260000
H	0.38783000	-0.80138300	1.98004200
H	-0.36803000	0.76874600	1.73587200
C	2.38525400	-0.78178200	-0.36314700
C	3.66304600	-0.32396800	-0.73204600
C	2.29210000	-2.08876500	0.14523400
C	4.78841500	-1.12727400	-0.58992400
H	3.76939500	0.67000400	-1.16309400
C	3.41732400	-2.89443000	0.28694300
H	1.31867400	-2.47623400	0.44094500
C	4.67514900	-2.41833400	-0.07535000
H	5.76082700	-0.74528500	-0.89383800
H	3.30989900	-3.89933800	0.69018900
H	5.55595400	-3.04590000	0.03751800
C	1.19565700	1.48280600	-0.32438200
C	2.15201300	2.08350300	0.52091900
C	0.13797700	3.52149600	-0.58409900
C	2.07436300	3.43840100	0.79640600
H	2.92824800	1.47712000	0.98015500
C	1.04710500	4.19202100	0.22925200
H	-0.68810000	4.06904400	-1.04228700
H	2.80315700	3.90223400	1.45761300
H	0.94716800	5.25770500	0.41416500
N	0.19392600	2.22024600	-0.85819200
C	-3.28623900	-1.92671100	-1.21034700
H	-2.29114700	-1.89842500	-1.66566600
H	-3.37361500	-2.81813100	-0.58448500
H	-4.01389400	-2.03457000	-2.02256600

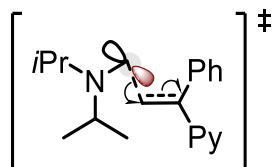
²⁷TS I₁-II₁

E = -887.384683

G_{Corr.} = 0.36641

C	-3.16181100	0.78631300	-2.01605900
C	-3.06681300	0.75559600	-0.48673000
H	-3.86136100	0.02476400	-2.38174200
H	-3.51872500	1.76727300	-2.35395400
H	-2.18711700	0.60662700	-2.48394600
C	-2.10232400	1.84059500	-0.00297100
H	-2.06045100	1.85567000	1.09376700
H	-1.08087800	1.70152000	-0.37617100
H	-2.44747800	2.82356900	-0.34645300
N	-2.57084700	-0.57379900	-0.02801400
C	-3.47474000	-1.622265400	0.47013300
C	-2.81364200	-2.45551300	1.56179200
C	-4.00851700	-2.50590200	-0.65469700
H	-4.32210300	-1.11429800	0.94020400
H	-2.38912600	-1.81352200	2.34190100
H	-3.56072700	-3.11206300	2.02199700
H	-2.01352300	-3.09717800	1.17156600
H	-4.58465900	-1.92530300	-1.38449200
H	-3.18284400	-2.99544000	-1.18757600
H	-4.66285400	-3.28906000	-0.25293900
C	-1.30340000	-0.95054100	-0.38109400
H	-1.09321900	-2.01475500	-0.45145200
H	-0.74177600	-0.30739000	-1.05216700
C	0.36836500	-0.58234800	1.37615000
H	-0.36586600	0.10203700	1.79263400
H	0.29730300	-1.61422000	1.71242000
C	1.48326000	-0.10754300	0.73916200
C	-4.44198000	1.06600400	0.09507000
H	-4.72519400	2.07884900	-0.21291200
H	-5.22198100	0.38717300	-0.26998500
H	-4.43379600	1.04384600	1.19191000
C	1.58257200	1.34130200	0.46181400
C	1.27882400	2.28274400	1.45409800
C	1.89284600	1.81544800	-0.82202400
C	1.26635000	3.64611200	1.17373000
H	1.05757800	1.93555700	2.46243500
C	1.87507500	3.17618500	-1.10658000
H	2.13586500	1.10222100	-1.60752600
C	1.55915700	4.09994400	-0.11033900
H	1.03253800	4.35693800	1.96367700
H	2.10704300	3.51860400	-2.11294500
H	1.54919100	5.16462300	-0.33235400
C	2.50846700	-1.02056800	0.22446600
C	2.24252200	-2.38954300	0.02094900
C	4.68807800	-1.32430000	-0.46586300
C	3.25452900	-3.22490100	-0.42200100
H	1.24515400	-2.78584500	0.19472700
C	4.51700400	-2.69059300	-0.67133300
H	5.65748100	-0.86208100	-0.65860100
H	3.05821800	-4.28267400	-0.58346200
H	5.33979900	-3.30659600	-1.02276200
N	3.72950100	-0.50675300	-0.03510600

²⁷TS I₂-II₂

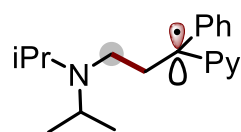


$$E = -887.389996$$

$$G_{\text{Corr.}} = 0.368372$$

N	-2.64373400	-0.28090900	0.61867800
C	-3.62222000	-0.64023000	-0.45972900
C	-3.68374600	0.47763500	-1.51338200
C	-4.99893600	-0.82705000	0.18365700
H	-2.70139300	0.65158600	-1.96946100
H	-4.37711700	0.18275900	-2.30984700
H	-4.04258200	1.42952800	-1.11076500
H	-4.97142800	-1.65275400	0.90527300
H	-5.34262400	0.07167500	0.70794000
H	-5.74517400	-1.06505500	-0.58489000
C	-1.45031200	-0.93861200	0.90543900
C	-0.00741000	-0.55873600	-0.94852200
H	-0.00900800	-1.59682100	-1.27644000
H	-0.81327900	0.07675700	-1.29745200
C	1.17949300	0.03800200	-0.57979200
C	-2.77440000	1.09309200	1.08834000
H	-2.13166600	1.79305500	0.52762200
H	-3.80894200	1.42508400	0.98729900
H	-2.52772600	1.16673200	2.14985000
C	-1.45051000	-2.44566600	1.02024100
H	-1.33636700	-2.98626200	0.07613500
H	-0.62170900	-2.75628500	1.66607600
H	-2.37976700	-2.79945300	1.49221100
C	-0.57717500	-0.28614200	1.93860200
H	-1.03059900	-0.35703600	2.94260000
H	0.38783000	-0.80138300	1.98004200
H	-0.36803000	0.76874600	1.73587200
C	2.38525400	-0.78178200	-0.36314700
C	3.66304600	-0.32396800	-0.73204600
C	2.29210000	-2.08876500	0.14523400
C	4.78841500	-1.12727400	-0.58992400
H	3.76939500	0.67000400	-1.16309400
C	3.41732400	-2.89443000	0.28694300
H	1.31867400	-2.47623400	0.44094500
C	4.67514900	-2.41833400	-0.07535000
H	5.76082700	-0.74528500	-0.89383800
H	3.30989900	-3.89933800	0.69018900
H	5.55595400	-3.04590000	0.03751800
C	1.19565700	1.48280600	-0.32438200
C	2.15201300	2.08350300	0.52091900
C	0.13797700	3.52149600	-0.58409900
C	2.07436300	3.43840100	0.79640600
H	2.92824800	1.47712000	0.98015500
C	1.04710500	4.19202100	0.22925200
H	-0.68810000	4.06904400	-1.04228700
H	2.80315700	3.90223400	1.45761300
H	0.94716800	5.25770500	0.41416500
N	0.19392600	2.22024600	-0.85819200
C	-3.28623900	-1.92671100	-1.21034700
H	-2.29114700	-1.89842500	-1.66566600
H	-3.37361500	-2.81813100	-0.58448500
H	-4.01389400	-2.03457000	-2.02256600

$^{27}\Pi_1$

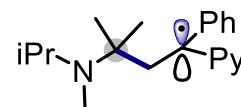


$$E = -887.4253372$$

$$G_{\text{Corr.}} = 0.37095$$

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C	-3.06681300	0.75559600	-0.48673000
H	-3.86136100	0.02476400	-2.38174200
H	-3.51872500	1.76727300	-2.35395400
H	-2.18711700	0.60662700	-2.48394600
C	-2.10232400	1.84059500	-0.00297100
H	-2.06045100	1.85567000	1.09376700
H	-1.08087800	1.70152000	-0.37617100
H	-2.44747800	2.82356900	-0.34645300
N	-2.57084700	-0.57379900	-0.02801400
C	-3.47474000	-1.62265400	0.47013300
C	-2.81364200	-2.45551300	1.56179200
C	-4.00851700	-2.50590200	-0.65469700
H	-4.32210300	-1.11429800	0.94020400
H	-2.38912600	-1.81352200	2.34190100
H	-3.56072700	-3.11206300	2.02199700
H	-2.01352300	-3.09717800	1.17156600
H	-4.58465900	-1.92530300	-1.38449200
H	-3.18284400	-2.99544000	-1.18757600
H	-4.66285400	-3.28906000	-0.25293900
C	-1.30340000	-0.95054100	-0.38109400
H	-1.09321900	-2.01475500	-0.45145200
H	-0.74177600	-0.30739000	-1.05216700
C	0.36836500	-0.58234800	1.37615000
H	-0.36586600	0.10203700	1.79263400
H	0.29730300	-1.61422000	1.71242000
C	1.48326000	-0.10754300	0.73916200
C	-4.44198000	1.06600400	0.09507000
H	-4.72519400	2.07884900	-0.21291200
H	-5.22198100	0.38717300	-0.26998500
H	-4.43379600	1.04384600	1.19191000
C	1.58257200	1.34130200	0.46181400
C	1.27882400	2.28274400	1.45409800
C	1.89284600	1.81544800	-0.82202400
C	1.26635000	3.64611200	1.17373000
H	1.05757800	1.93555700	2.46243500
C	1.87507500	3.17618500	-1.10658000
H	2.13586500	1.10222100	-1.60752600
C	1.55915700	4.09994400	-0.11033900
H	1.03253800	4.35693800	1.96367700
H	2.10704300	3.51860400	-2.11294500
H	1.54919100	5.16462300	-0.33235400
C	2.50846700	-1.02056800	0.22446600
C	2.24252200	-2.38954300	0.02094900
C	4.68807800	-1.32430000	-0.46586300
C	3.25452900	-3.22490100	-0.42200100
H	1.24515400	-2.78584500	0.19472700
C	4.51700400	-2.69059300	-0.67133300
H	5.65748100	-0.86208100	-0.65860100
H	3.05821800	-4.28267400	-0.58346200
H	5.33979900	-3.30659600	-1.02276200
N	3.72950100	-0.50675300	-0.03510600

$^{27}\Pi_2$



$$E = -887.4227282$$

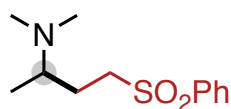
$$G_{\text{Corr.}} = 0.374989$$

N	-2.64373400	-0.28090900	0.61867800
C	-3.62222000	-0.64023000	-0.45972900
C	-3.68374600	0.47763500	-1.51338200
C	-4.99893600	-0.82705000	0.18365700
H	-2.70139300	0.65158600	-1.96946100
H	-4.37711700	0.18275900	-2.30984700
H	-4.04258200	1.42952800	-1.11076500
H	-4.97142800	-1.65275400	0.90527300
H	-5.34262400	0.07167500	0.70794000

H	-5.74517400	-1.06505500	-0.58489000	H	3.76939500	0.67000400	-1.16309400
C	-1.45031200	-0.93861200	0.90543900	C	3.41732400	-2.89443000	0.28694300
C	-0.00741000	-0.55873600	-0.94852200	H	1.31867400	-2.47623400	0.44094500
H	-0.00900800	-1.59682100	-1.27644000	C	4.67514900	-2.41833400	-0.07535000
H	-0.81327900	0.07675700	-1.29745200	H	5.76082700	-0.74528500	-0.89383800
C	1.17949300	0.03800200	-0.57979200	H	3.30989900	-3.89933800	0.69018900
C	-2.77440000	1.09309200	1.08834000	H	5.55595400	-3.04590000	0.03751800
H	-2.13166600	1.79305500	0.52762200	C	1.19565700	1.48280600	-0.32438200
H	-3.80894200	1.42508400	0.98729900	C	2.15201300	2.08350300	0.52091900
H	-2.52772600	1.16673200	2.14985000	C	0.13797700	3.52149600	-0.58409900
C	-1.45051000	-2.44566600	1.02024100	C	2.07436300	3.43840100	0.79640600
H	-1.33636700	-2.98626200	0.07613500	H	2.92824800	1.47712000	0.98015500
H	-0.62170900	-2.75628500	1.66607600	C	1.04710500	4.19202100	0.22925200
H	-2.37976700	-2.79945300	1.49221100	H	-0.68810000	4.06904400	-1.04228700
C	-0.57717500	-0.28614200	1.93860200	H	2.80315700	3.90223400	1.45761300
H	-1.03059900	-0.35703600	2.94260000	H	0.94716800	5.25770500	0.41416500
H	0.38783000	-0.80138300	1.98004200	N	0.19392600	2.22024600	-0.85819200
H	-0.36803000	0.76874600	1.73587200	C	-3.28623900	-1.92671100	-1.21034700
C	2.38525400	-0.78178200	-0.36314700	H	-2.29114700	-1.89842500	-1.66566600
C	3.66304600	-0.32396800	-0.73204600	H	-3.37361500	-2.81813100	-0.58448500
C	2.29210000	-2.08876500	0.14523400	H	-4.01389400	-2.03457000	-2.02256600
C	4.78841500	-1.12727400	-0.58992400				

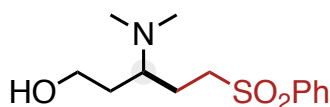
V. α -C(sp³)-H alkylation by dynamic radical trapping

General Procedure A for Alkylation: A 8.0 mL disposable borosilicate glass tube with screw cap containing a stirring bar was charged with TPS-SH (10 mol%, 5.9 mg, 0.02 mmol), Ir(ppy)₂(dtbbpy)PF₆ (1 mol%, 1.8 mg, 0.002 mmol), trialkylamine (0.6 mmol, added after solvent if volatile liquid) and olefin (0.2 mmol, added after solvent if liquid). The tube was transferred to a nitrogen-filled glove-box where the dry Tol (2.0 mL, 0.1 M) was added. Then the reaction was stirred for 1 minute and transferred outside, placing ~10 cm away from a Kessil blue LED (34W maximum, 24 VDC) and rigorously stirred for the mentioned time (4~16 h) with cooling by fan. After completion of the reaction, the product was directly purified by flash column chromatography in silica gel with CHCl₃/MeOH.



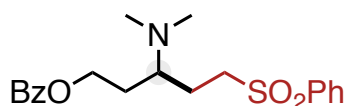
6

***N,N*-dimethyl-4-(phenylsulfonyl)butan-2-amine:** Following the general procedure A, the title compound was obtained in 86% yield after 4 h as colorless oil. ¹H NMR (400 MHz, CDCl₃) δ 7.92-7.90 (m, 2H), 7.65-7.62 (m, 1H), 7.57-7.53 (m, 2H), 3.30-3.23 (m, 1H), 3.15-3.07 (m, 1H), 2.60-2.51 (m, 1H), 2.10 (s, 6H), 1.81-1.72 (m, 2H), 0.90 (d, J = 6.5 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 139.65, 133.77, 129.45, 128.19, 57.71, 53.85, 40.25, 26.80, 12.71. IR (CDCl₃, cm⁻¹): 3063, 2960, 2928, 1447, 1304, 1286, 1086, 737. HRMS *calcd.* for (C₁₂H₂₀NO₂S) [M+H]⁺: 242.1215, *found* 242.1238.



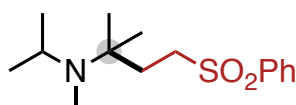
7

3-(dimethylamino)-5-(phenylsulfonyl)pentan-1-ol: Following the general procedure A, the title compound was obtained in 53% yield after 8 h as colorless oil. ¹H NMR (400 MHz, CDCl₃) δ 7.92-7.90 (m, 2H), 7.69-7.65 (m, 1H), 7.60-7.56 (m, 2H), 3.76-3.68 (m, 2H), 3.13-3.04 (m, 2H), 2.78-2.71 (m, 1H), 2.27 (s, 6H), 2.08-1.99 (m, 1H), 1.81-1.71 (m, 1H), 1.71-1.60 (m, 1H), 1.38-1.32 (m, 1H), 1.04 (s, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 139.34, 133.99, 129.53, 128.06, 63.74, 62.76, 54.31, 40.03, 30.78, 20.52. IR (CDCl₃, cm⁻¹): 3372, 3061, 2943, 2781, 1306, 1083, 739, 690. HRMS *calcd.* for (C₁₃H₂₂NO₃S) [M+H]⁺: 272.1320, *found* 272.1323.



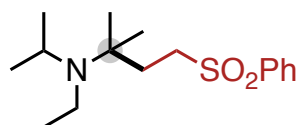
8

3-(dimethylamino)-5-(phenylsulfonyl)pentyl benzoate: Following the general procedure A, the title compound was obtained in 86% yield after 8 h as yellow oil. ^1H NMR (500 MHz, CDCl_3) δ 8.06 (d, $J = 7.4$ Hz, 2H), 7.58 (t, $J = 7.3$ Hz, 1H), 7.46 (t, $J = 7.5$ Hz, 2H), 4.44-4.37 (m, 2H), 2.62-2.26 (m, 9H), 2.00-1.93 (m, 1H), 1.85-1.60 (m, 3H), 1.46 (s, 9H). ^{13}C NMR (126 MHz, CDCl_3) δ 173.19, 166.67, 132.93, 130.52, 129.61, 128.43, 80.14, 63.41, 60.33, 40.26, 33.11, 28.20, 25.06. IR (CDCl_3 , cm^{-1}): 3064, 2966, 2931, 1718, 1452, 1270, 1147, 710. IR (CDCl_3 , cm^{-1}): 3060, 3028, 2934, 1727, 1436, 1278, 970, 687. HRMS *calcd.* for ($\text{C}_{20}\text{H}_{26}\text{NO}_4\text{S}$) $[\text{M}+\text{H}]^+$: 376.1583, *found* 376.1578.



9

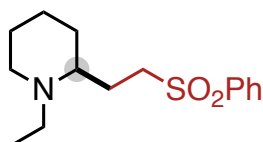
***N*-isopropyl-*N*,2-dimethyl-4-(phenylsulfonyl)butan-2-amine:** Following the general procedure A, the title compound was obtained in 86% yield after 8 h as colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 7.91 (d, $J = 7.3$ Hz, 2H), 7.64 (t, $J = 7.4$ Hz, 1H), 7.56 (t, $J = 7.5$ Hz, 2H), 3.19-3.15 (m, 2H), 3.04 (dt, $J = 12.9, 6.4$ Hz, 1H), 1.97 (s, 3H), 1.77-1.73 (m, 2H), 0.98 (s, 6H), 0.90 (d, $J = 6.5$ Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 139.66, 133.58, 129.31, 128.08, 56.10, 52.39, 45.79, 33.66, 26.63, 24.94, 21.06. IR (CDCl_3 , cm^{-1}): 2970, 2876, 2788, 1462, 1292, 1086, 955, 742. HRMS *calcd.* for ($\text{C}_{15}\text{H}_{26}\text{NO}_2\text{S}$) $[\text{M}+\text{H}]^+$: 284.1684, *found* 284.1691.



10

***N*-ethyl-*N*-isopropyl-2-methyl-4-(phenylsulfonyl)butan-2-amine:** Following the general procedure A, the title compound was obtained in 38% yield after 8 h as yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 7.93-7.91 (m, 2H), 7.67-7.63 (m, 1H), 7.59-7.55 (m, 3H), 3.24-3.19 (m, 2H), 3.00 (p, $J = 6.6$ Hz, 1H), 2.46 (q, $J = 7.0$ Hz, 2H), 1.77-1.73 (m, 2H), 1.01 (s, 6H), 0.93 (d, $J = 6.6$ Hz, 6H), 0.91 (t, $J = 7.1$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 139.72, 133.61, 129.35, 128.15, 57.09, 52.63, 46.48, 35.34, 34.32, 26.56, 22.49, 20.27. IR (CDCl_3 , cm^{-1}): 2970, 2927, 2872, 1446, 1303, 1087, 743, 689. HRMS *calcd.* for ($\text{C}_{16}\text{H}_{28}\text{NO}_2\text{S}$) $[\text{M}+\text{H}]^+$: 298.1841, *found* 298.1853.

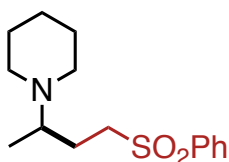
Note: ratio was obtained by GC-MS, the other regioisomer decomposed during purification.



65

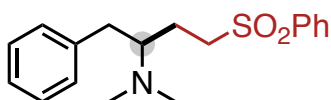
11

1-ethyl-2-(2-(phenylsulfonyl)ethyl)piperidine: Following the general procedure A, the title compound was obtained in 53% yield after 8 h as colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 7.91 (d, $J = 7.1$ Hz, 2H), 7.65 (t, $J = 7.4$ Hz, 1H), 7.56 (t, $J = 7.5$ Hz, 2H), 3.24-3.06 (m, 2H), 2.82 (d, $J = 11.6$ Hz, 1H), 2.65-2.56 (m, 1H), 2.37-2.26 (m, 2H), 2.15 (t, $J = 10.7$ Hz, 1H), 2.04-1.96 (m, 1H), 1.89-1.82 (m, 1H), 1.65-1.37 (m, 4H), 1.29-1.19 (m, 2H), 0.94 (t, $J = 7.0$ Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 139.47, 133.74, 129.38, 128.13, 57.77, 52.32, 51.02, 46.65, 30.06, 25.14, 24.40, 23.78, 10.60. IR (CDCl_3 , cm^{-1}): 2930, 2855, 2796, 1446, 1304, 1086, 732, 689. HRMS *calcd.* for ($\text{C}_{15}\text{H}_{24}\text{NO}_2\text{S}$) $[\text{M}+\text{H}]^+$: 282.1528, *found* 282.1537.



11'

1-(4-(phenylsulfonyl)butan-2-yl)piperidine: Following the general procedure A, the title compound was obtained in 23% yield after 8 h as colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 7.92 (d, $J = 7.3$ Hz, 2H), 7.65 (t, $J = 7.4$ Hz, 1H), 7.57 (t, $J = 7.6$ Hz, 2H), 3.39-3.32 (m, 1H), 3.18-3.10 (m, 1H), 2.57-2.16 (m, 5H), 1.85-1.64 (m, 2H), 1.49-1.38 (m, 6H), 0.90 (d, $J = 6.0$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 139.63, 133.63, 129.36, 128.13, 58.20, 53.94, 49.12, 26.71, 26.53, 24.94, 13.45. IR (CDCl_3 , cm^{-1}): 2932, 2851, 2798, 1446, 1303, 1144, 1086, 744. HRMS *calcd.* for ($\text{C}_{15}\text{H}_{24}\text{NO}_2\text{S}$) $[\text{M}+\text{H}]^+$: 282.1528, *found* 282.1536.



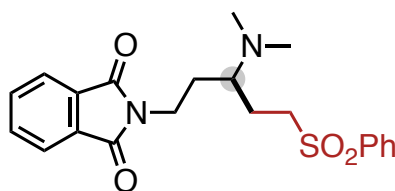
12

***N,N*-dimethyl-1-phenyl-4-(phenylsulfonyl)butan-2-amine:** Following the general procedure A, the title compound was obtained in 70% yield after 8 h as colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 7.78 (d, $J = 8.1$ Hz, 2H), 7.60 (t, $J = 7.4$ Hz, 1H), 7.49 (t, $J = 7.6$ Hz, 2H), 7.28-7.24 (m, 2H), 7.21-7.17 (m, 1H), 7.08-7.07 (m, 2H), 3.31-3.24 (m, 1H), 3.01-2.94 (m, 2H), 2.64-2.58 (m, 1H), 2.23 (s, 6H), 2.23-2.18 (m, 1H), 1.77-1.71 (m, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ 139.79, 139.47, 133.51, 129.25, 129.21, 128.68, 128.08, 126.23, 64.74, 53.67, 40.11, 33.53, 23.73. IR (CDCl_3 , cm^{-1}): 3099, 3060, 3028, 2934, 1506, 1086, 738, 690. HRMS *calcd.* for ($\text{C}_{18}\text{H}_{24}\text{NO}_2\text{S}$) $[\text{M}+\text{H}]^+$: 318.1528, *found* 318.1546.

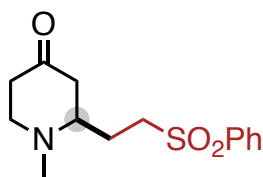


13 (5:1)

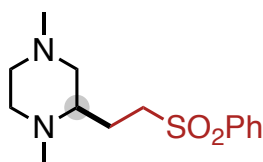
6-(*tert*-butyl) 1-methyl 3-(dimethylamino)hexanedioate (major) : Following the general procedure A, the title compound was obtained in 89% yield after 8 h as a mixture of yellow oil. ¹H NMR (500 MHz, CDCl₃) δ 3.64 (s, 3H), 2.93-2.18 (m, 11H), 1.72-1.56 (m, 2H), 1.41 (s, 9H). ¹³C NMR (126 MHz, CDCl₃) δ 173.52, 173.07, 80.09, 60.58, 51.75, 40.19, 33.47, 32.90, 28.19, 26.59. IR (CDCl₃, cm⁻¹): 2932, 2867, 1728, 1454, 1366, 1223, 1148, 1044. IR (CDCl₃, cm⁻¹): 2945, 2781, 1731, 1723, 1446, 1254, 1227, 845. HRMS *calcd.* for (C₁₃H₂₆NO₄) [M+H]⁺: 260.1862, *found* 260.1873.

**14**

2-(3-(dimethylamino)-5-(phenylsulfonyl)pentyl)isoindoline-1,3-dione: Following the general procedure A, the title compound was obtained in 82% yield after 8 h as colorless oil. ¹H NMR (400 MHz, CDCl₃) δ 7.93-7.91 (m, 2H), 7.83-7.80 (m, 2H), 7.73-7.69 (m, 2H), 7.66-7.62 (m, 1H), 7.58-7.54 (m, 2H), 3.68-3.65 (m, 2H), 3.29-3.21 (m, 1H), 3.16-3.08 (m, 1H), 2.48 (br, 1H), 2.14 (s, 6H), 1.93-1.78 (m, 3H), 1.51-1.42 (m, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 168.39, 139.52, 134.09, 133.74, 132.23, 129.41, 128.12, 123.35, 60.52, 53.98, 40.02, 36.07, 27.55, 22.89. IR (CDCl₃, cm⁻¹): 2937, 2826, 2780, 1770, 1707, 1397, 1146, 720. HRMS *calcd.* for (C₂₁H₂₅N₂O₄S) [M+H]⁺: 401.1535, *found* 401.1539.

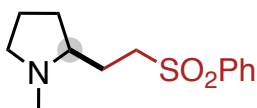
**15**

1-methyl-2-(2-(phenylsulfonyl)ethyl)piperidin-4-one: Following the general procedure A, the title compound was obtained in 72% yield after 8 h as colorless oil. ¹H NMR (400 MHz, CDCl₃) δ 7.91-7.89 (m, 2H), 7.68-7.64 (m, 1H), 7.59-7.55 (m, 2H), 3.24-3.12 (m, 2H), 3.09-3.03 (m, 1H), 2.69-2.57 (m, 2H), 2.48-2.15 (m, 8H), 2.01-1.92 (m, 1H), 1.89-1.80 (m, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 207.80, 139.17, 133.95, 129.50, 128.08, 60.75, 53.57, 44.01, 39.91, 39.67, 25.50. IR (CDCl₃, cm⁻¹): 2956, 2795, 1714, 1446, 1303, 1085, 915, 730. HRMS *calcd.* for (C₁₄H₂₀NO₃S) [M+H]⁺: 282.1164, *found* 282.1171.



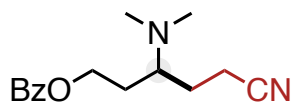
16

1,4-dimethyl-2-(2-(phenylsulfonyl)ethyl)piperazine: Following the general procedure A, the title compound was obtained in 73% yield after 8 h as colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 7.90 (d, $J = 7.8$ Hz, 2H), 7.65 (t, $J = 7.4$ Hz, 1H), 7.56 (t, $J = 7.6$ Hz, 2H), 3.27-3.19 (m, 1H), 3.09-3.01 (m, 1H), 2.72-2.63 (m, 2H), 2.29 (td, $J = 11.3, 2.8$ Hz, 1H), 2.21 (s, 3H), 2.12 (s, 3H), 2.08-1.94 (m, 2H), 1.86-1.76 (m, 2H). ^{13}C NMR (126 MHz, CDCl_3) δ 139.18, 133.84, 129.43, 128.15, 59.92, 59.07, 55.40, 54.92, 51.81, 46.07, 42.10, 23.36. IR (CDCl_3 , cm^{-1}): 3062, 2937, 2795, 2795, 1446, 1300, 1143, 734. HRMS *calcd.* for ($\text{C}_{14}\text{H}_{23}\text{N}_2\text{O}_2\text{S}$) $[\text{M}+\text{H}]^+$: 283.1480, *found* 283.1489.



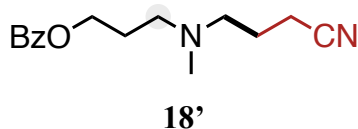
17

1-methyl-2-(2-(phenylsulfonyl)ethyl)pyrrolidine: Following the general procedure A, the title compound was obtained in 69% yield after 8 h as colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 7.91 (d, $J = 8.0$ Hz, 2H), 7.65 (t, $J = 7.9$ Hz, 1H), 7.56 (t, $J = 7.7$ Hz, 2H), 3.23-3.15 (m, 1H), 3.10-3.02 (m, 2H), 2.25-2.15 (m, 5H), 2.08-2.00 (m, 1H), 1.92-1.83 (m, 1H), 1.79-1.65 (m, 3H), 1.42-1.33 (m, 1H). ^{13}C NMR (126 MHz, CDCl_3) δ 139.18, 133.81, 129.42, 128.17, 64.15, 57.14, 52.87, 40.31, 29.85, 25.66, 22.06. IR (CDCl_3 , cm^{-1}): 3062, 2945, 2781, 1446, 1303, 1086, 739, 689. HRMS *calcd.* for ($\text{C}_{13}\text{H}_{20}\text{NO}_2\text{S}$) $[\text{M}+\text{H}]^+$: 254.1215, *found* 254.1219.

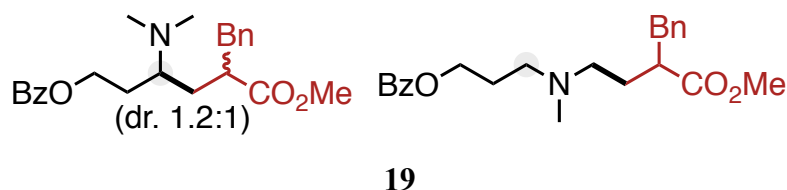


18

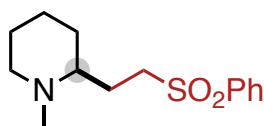
5-cyano-3-(dimethylamino)pentyl benzoate: Following the general procedure A, the title compound was obtained in 72% yield after 8 h as colorless oil. ^1H NMR (500 MHz, CDCl_3) δ 8.03-8.02 (m, 2H), 7.57-7.54 (m, 1H), 7.46-7.42 (m, 2H), 4.40-4.32 (m, 2H), 2.73-2.67 (m, 1H), 2.45 (t, $J = 7.3$ Hz, 13H), 2.24 (s, 6H), 2.09-2.02 (m, 1H), 1.80-1.74 (m, 2H), 1.59 (d, $J = 34.9$ Hz, 1H). ^{13}C NMR (126 MHz, CDCl_3) δ 166.58, 133.11, 130.21, 129.59, 128.52, 120.08, 62.98, 59.56, 40.03, 26.89, 26.83, 14.62. IR (CDCl_3 , cm^{-1}): 2938, 2826, 2781, 2240, 1715, 1452, 1272, 713. HRMS *calcd.* for ($\text{C}_{15}\text{H}_{21}\text{N}_2\text{O}_2$) $[\text{M}+\text{H}]^+$: 261.1603, *found* 261.1610.



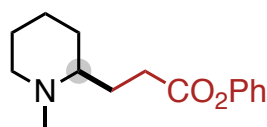
3-((3-cyanopropyl)(methyl)amino)propyl benzoate: Following the general procedure A, the title compound was obtained in 14% yield after 8 h as colorless oil. ^1H NMR (500 MHz, CDCl_3) δ 8.04-8.03 (m, 2H), 7.58-7.54 (m, 1H), 7.46-7.43 (m, 2H), 4.38 (t, $J = 6.5$ Hz, 2H), 2.49 (dt, $J = 15.0, 6.8$ Hz, 4H), 2.41 (t, $J = 7.1$ Hz, 2H), 2.22 (s, 3H), 1.93 (p, $J = 6.7$ Hz, 2H), 1.80 (p, $J = 6.9$ Hz, 2H). ^{13}C NMR (126 MHz, CDCl_3) δ 166.72, 133.05, 130.45, 129.65, 128.52, 119.95, 63.22, 55.81, 54.36, 41.93, 26.81, 23.57, 14.85. IR (CDCl_3 , cm^{-1}): 2955, 2801, 2246, 1716, 1452, 1274, 1115, 713. HRMS *calcd.* for ($\text{C}_{15}\text{H}_{21}\text{N}_2\text{O}_2$) [$\text{M}+\text{H}$] $^+$: 261.1603, *found* 261.1600.



5-benzyl-3-(dimethylamino)-6-methoxy-6-oxohexyl benzoate (major): Following the general procedure A, the title compound was obtained in 81% yield after 8 h as a mixture of yellow oil. Selected peaks for: ^1H NMR (500 MHz, CDCl_3) δ 8.05-8.08 (m, 2H), 7.57-7.60 (m, 1H), 7.45-7.48 (m, 2H), 7.28-7.31 (m, 2H), 7.17-7.23 (m, 3H), 4.30-4.41 (m, 2H). ^{13}C NMR (126 MHz, CDCl_3) δ 176.02, 166.59, 139.25, 132.97, 130.45, 129.60, 128.97, 128.92, 128.45, 126.44, 63.19, 59.26, 51.32, 40.06. IR (CDCl_3 , cm^{-1}): 2948, 2840, 1718, 1602, 1452, 1272, 1113, 712. HRMS *calcd.* for ($\text{C}_{23}\text{H}_{30}\text{NO}_4$) [$\text{M}+\text{H}$] $^+$: 384.2175, *found* 384.2167.

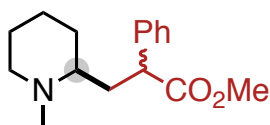


1-methyl-2-(2-(phenylsulfonyl)ethyl)piperidine: Following the general procedure A, the title compound was obtained in 86% yield after 4 h as colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 7.91 (d, $J = 7.9$ Hz, 2H), 7.64 (t, $J = 7.4$ Hz, 1H), 7.56 (t, $J = 7.7$ Hz, 2H), 3.27-3.19 (m, 1H), 3.12-3.04 (m, 1H), 2.78 (d, $J = 11.6$ Hz, 1H), 2.11 (s, 3H), 2.06-2.00 (m, 3H), 1.87-1.80 (m, 1H), 1.69-1.64 (m, 1H), 1.57-1.40 (m, 3H), 1.27-1.16 (m, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ 139.44, 133.75, 129.38, 128.14, 61.59, 57.05, 51.81, 42.74, 30.36, 25.63, 25.46, 24.33. IR (CDCl_3 , cm^{-1}): 3062, 2928, 2854, 1446, 1304, 1284, 1086, 689. HRMS *calcd.* for ($\text{C}_{14}\text{H}_{22}\text{NO}_2\text{S}$) [$\text{M}+\text{H}$] $^+$: 268.1371, *found* 268.1376.



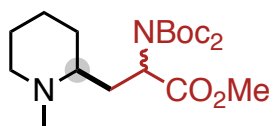
21

phenyl 3-(1-methylpiperidin-2-yl)propanoate: Following the general procedure A, the title compound was obtained in 76% yield after 8 h as colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 7.39-7.35 (m, 2H), 7.24-7.20 (m, 1H), 7.09-7.06 (2H), 3.07 (d, $J = 10.2$ Hz, 1H), 2.79-2.71 (m, 1H), 2.65-2.39 (m, 6H), 2.19-2.12 (m, 1H), 2.06-1.97 (m, 1H), 1.87-1.68 (m, 4H), 1.62-1.51 (m, 1H), 1.41-1.35 (m, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 172.05, 150.74, 129.58, 126.02, 121.61, 63.16, 56.72, 41.95, 29.98, 29.16, 26.81, 24.47, 23.46. IR (CDCl_3 , cm^{-1}): 2935, 2855, 1756, 1592, 1491, 1194, 1136, 752. HRMS *calcd.* for ($\text{C}_{15}\text{H}_{22}\text{NO}_2$) $[\text{M}+\text{H}]^+$: 248.1651, *found* 248.1671.



22 (~dr. 1.2:1)

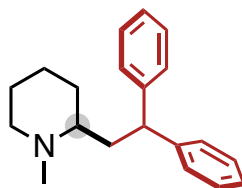
methyl 3-(1-methylpiperidin-2-yl)-2-phenylpropanoate: Following the general procedure A, the title compound was obtained in 69% yield (~dr. 1.2:1) after 8 h as colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 7.33-7.23 (m, 5H), 3.74-3.62 (m, 4H), 2.98-2.95 (m, 0.53H), 2.91-2.88 (m, 0.43H), 2.65-1.60 (m, 11H), 1.47-1.20 (m, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ (174.21, 174.15), (139.23, 138.25), (128.94, 128.90), 128.06, 127.79, (127.65, 127.54), (62.20, 61.43), (56.24, 55.96), (52.28, 52.25), (48.40, 47.90), (42.27, 41.92), (35.78, 34.65), (29.82, 29.34), (24.59, 24.39), (23.24, 23.03). IR (CDCl_3 , cm^{-1}): 3028, 2934, 2855, 1731, 1452, 1203, 733, 699. HRMS *calcd.* for ($\text{C}_{16}\text{H}_{24}\text{NO}_2$) $[\text{M}+\text{H}]^+$: 262.1807, *found* 262.1825.



23 (~dr. 1.2:1)

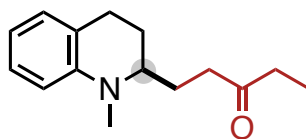
methyl 2-(bis(*tert*-butoxycarbonyl)amino)-3-(1-methylpiperidin-2-yl)propanoate: Following the general procedure A, the title compound was obtained in 81% yield (~dr. 1.2:1) after 8 h as colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 4.96, 4.88 (m, 1H), 3.68 (two single, 3H), 2.92-2.83 (m, 1H), 2.72-2.03 (m, 6H), 1.85-1.20 (m, 25H). ^{13}C NMR (101 MHz, CDCl_3) δ 171.53, (152.19, 151.99), (83.35, 83.34), (61.44, 60.90), (56.32, 56.25), (55.86, 55.60), (52.39, 52.32), (42.76, 42.37), (33.45, 31.83), (30.43, 30.31), 28.07, (25.22, 24.72), 23.37. IR (CDCl_3 ,

cm⁻¹): 2978, 2933, 1793, 1743, 1699, 1365, 994, 852. HRMS *calcd.* for (C₂₀H₃₇N₂O₆) [M+H]⁺: 401.2652, *found* 401.2665.



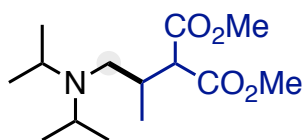
24

2-(2,2-diphenylethyl)-1-methylpiperidine: Following the general procedure B, 50 mol% of 2-*tert*-butyl-1,1,3,3-tetramethylguanidine (Barton's base) was used in Tol (0.1 M), the title compound was obtained in 74% yield after 8 h as yellow oil. ¹H NMR (400 MHz, CDCl₃) δ 7.34-7.15 (m, 10H), 4.02 (dd, *J* = 10.9, 5.1 Hz, 1H), 3.19 (d, *J* = 11.9 Hz, 1H), 2.75-2.56 (m, 3H), 2.60 (s, 3H), 2.34-2.27 (m, 1H), 2.01-1.90 (m, 2H), 1.79-1.71 (m, 3H), 1.36-1.25 (m, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 143.90, 142.19, 129.13, 128.81, 127.98, 127.59, 127.12, 126.78, 62.59, 55.29, 47.75, 40.25, 35.86, 27.49, 22.56, 21.78. IR (CDCl₃, cm⁻¹): 3057, 3025, 2935, 1451, 1439, 841, 751, 702. HRMS *calcd.* for (C₂₀H₂₆N) [M+H]⁺: 280.2065, *found* 280.2086.



25

1-(1-methyl-1,2,3,4-tetrahydroquinolin-2-yl)pentan-3-one: Following the general procedure A, the title compound was obtained in 46% yield after 8 h as colorless oil. ¹H NMR (400 MHz, CDCl₃) δ 7.09 (t, *J* = 7.6 Hz, 1H), 6.97 (d, *J* = 7.2 Hz, 1H), 6.60 (t, *J* = 7.3 Hz, 1H), 6.55 (d, *J* = 8.1 Hz, 1H), 3.26 (dq, *J* = 8.6, 4.4 Hz, 1H), 2.95 (s, 3H), 2.84-2.75 (m, 1H), 2.71-2.64 (m, 1H), 2.44 (q, *J* = 7.3 Hz, 3H), 1.99-1.80 (m, 3H), 1.73-1.63 (m, 1H), 1.07 (t, *J* = 7.3 Hz, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 211.18, 145.41, 128.77, 127.28, 121.96, 115.74, 111.02, 58.18, 38.67, 38.28, 36.09, 25.73, 24.64, 23.77, 7.99. IR (CDCl₃, cm⁻¹): 3019, 2935, 1712, 1454, 1500, 1337, 1215, 745. HRMS *calcd.* for (C₁₅H₂₂NO) [M+H]⁺: 232.1701, *found* 232.1707.

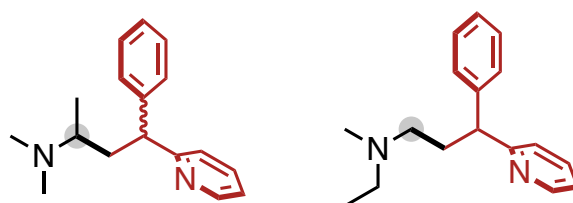


26

dimethyl 2-(1-(diisopropylamino)propan-2-yl)malonate: Following the general procedure A, the title compound was obtained in 73% yield after 8 h as colorless oil. ¹H NMR (400 MHz, CDCl₃) δ 4.19-4.13 (m, 4H), 3.49 (d, *J* = 5.8 Hz, 1H), 2.96 (hept, *J* = 6.7 Hz, 2H), 2.43-2.36

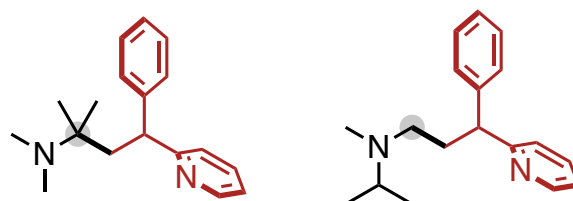
(m, 1H), 2.33-2.24 (m, 2H), 1.24 (t, $J = 7.1$ Hz, 7H), 0.97 (d, $J = 6.5$ Hz, 3H), 0.94 (d, $J = 6.7$ Hz, 15H). ^{13}C NMR (101 MHz, CDCl_3) δ 169.97, 169.20, 61.10, 60.93, 54.39, 49.16, 47.43, 32.82, 21.02, 20.64, 15.14, 14.22. IR (CDCl_3 , cm^{-1}): 2965, 2934, 1728, 1462, 1365, 1228, 1152, 1030. HRMS *calcd.* for ($\text{C}_{14}\text{H}_{28}\text{NO}_4$) $[\text{M}+\text{H}]^+$: 274.2018, *found* 274.2022.

General Procedure B for amino alkylation of diary styrene: A 8.0 mL disposable borosilicate glass tube with screw cap containing a stirring bar was charged with TPS-SH (5 mol%, 2.9 mg, 0.01 mmol), $\text{Ir}(\text{ppy})_2(\text{dtbbpy})\text{PF}_6$ (1 mol%, 1.8 mg, 0.002 mmol), trialkylamine (0.6 mmol, added after solvent if volatile liquid) and diary styrene (0.2 mmol, added after solvent if liquid). The tube was transferred to a nitrogen-filled glove-box where the dry 1,4-Dioxane (2.0 mL, 0.1 M) was added. Then the reaction was stirred for 1 minute and transferred outside, placing ~10 cm away from a 34 W Blue-Leds and rigorously stirred for 8h with cooling by fan. After completion of the reaction, the product was directly purified by flash column chromatography in silica gel with $\text{CHCl}_3/\text{MeOH}$.



27 (2.6:1)

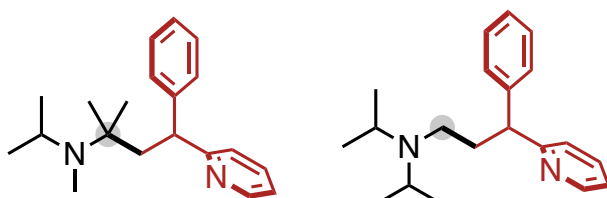
***N,N*-dimethyl-4-phenyl-4-(pyridin-2-yl)butan-2-amine** (major): Following the general procedure B, the title compound was obtained in 91% as a mixture of yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 8.57-8.55 (m, 1H), 7.56-7.51 (m, 1H), 7.39-7.34 (m, 2H), 7.30-7.25 (m, 2H), 7.20-7.15 (m, 2H), 7.08-7.04 (m, 1H), 4.30-4.23 (m, 0.73H), 4.15-4.11 (m, 0.28H), 2.51-1.92 (m, 9H), 1.00-0.94 (m, 3H). Selected peaks: ^{13}C NMR (101 MHz, CDCl_3) δ 149.20, 136.34, 128.56, 128.48, 128.20, 126.05, 123.55, 120.99, 49.42, 27.04, 26.11, 25.55, 21.31, 21.01. IR (CDCl_3 , cm^{-1}): 3060, 2962, 1587, 1469, 1431, 1047, 747, 699. HRMS *calcd.* for ($\text{C}_{17}\text{H}_{23}\text{N}_2$) $[\text{M}+\text{H}]^+$: 255.1861, *found* 255.1857.



28 (1.3:1)

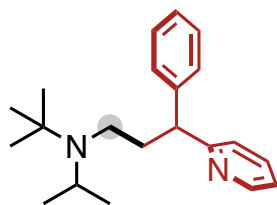
***N,N*,2-trimethyl-4-phenyl-4-(pyridin-2-yl)butan-2-amine** (major): Following the general procedure B, the title compound was obtained in 88% as a mixture of yellow oil. Selected peaks for ^1H NMR (400 MHz, CDCl_3) δ 8.5-8.53 (m, 2.3H), 4.40 (m, 1.3H), 4.16 (t, $J = 7.5$ Hz,

1H), 0.92 (d, $J = 6.6$ Hz, 6H), 0.87 (s, 3.9H), 0.86 (s, 3.9H). ^{13}C NMR (101 MHz, CDCl_3) δ 164.88, 163.88, 149.27, 149.15, 146.16, 143.86, 136.43, 136.40, 135.20, 129.77, 128.54, 128.50, 128.47, 128.14, 128.08, 127.81, 126.45, 126.12, 123.50, 122.88, 121.31, 121.07, 56.91, 53.46, 51.55, 51.44, 48.87, 43.85, 38.54, 36.90, 32.99, 24.10, 22.67, 18.08, 17.75. IR (CDCl_3 , cm^{-1}): 3061, 3025, 2973, 1469, 1430, 1047, 747, 700. HRMS *calcd.* for ($\text{C}_{18}\text{H}_{25}\text{N}_2$) $[\text{M}+\text{H}]^+$: 269.2018, *found* 269.2029.



29 (2:1)

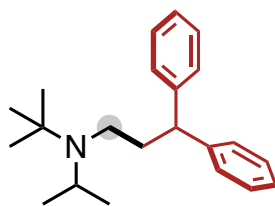
***N*-isopropyl-*N*,2-dimethyl-4-phenyl-4-(pyridin-2-yl)butan-2-amine** (major): Following the general procedure B, the title compound was obtained in 68% as a mixture of yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 8.56-8.54 (m, 1.5H), 7.56-7.00 (m, 12H), 4.40-4.37 (m, 1H), 4.16-4.12 (m, 0.5H), 3.27-3.21 (m, 1H), 3.03-3.00 (m, 1H), 2.75-2.70 (m, 1H), 2.49-2.41 (m, 1.5H), 2.19-2.13 (m, 1.5H), 2.08 (s, 3H), 1.01-0.88 (m, 18H). Selected peaks: ^{13}C NMR (101 MHz, CDCl_3) δ 149.20, 136.34, 128.56, 128.48, 128.20, 126.05, 123.55, 120.99, 49.42, 27.04, 26.11, 25.55, 21.31, 21.01. IR (CDCl_3 , cm^{-1}): 3024, 2966, 2872, 1587, 1469, 1431, 746, 699. HRMS *calcd.* for ($\text{C}_{20}\text{H}_{29}\text{N}_2$) $[\text{M}+\text{H}]^+$: 297.2331, *found* 297.2333.



30

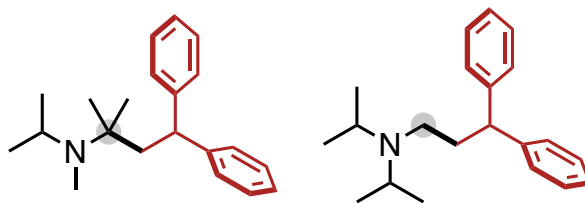
***N*-(*tert*-butyl)-*N*-isopropyl-3-phenyl-3-(pyridin-2-yl)propan-1-amine**: Following the general procedure B, the title compound was obtained in 95% as yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 8.55-8.53 (m, 1H), 7.56-7.52 (m, 1H), 7.38-7.35 (m, 2H), 7.30-7.28 (m, 2H), 7.20-7.15 (m, 2H), 7.07-7.04 (m, 1H), 4.06 (t, $J = 7.4$ Hz, 1H), 3.34 (br, 1H), 2.46 (br, 3H), 2.23 (br, 1H), 1.05 (s, 9H), 0.95 (s, 6H). Selected peaks for ^{13}C NMR (101 MHz, CDCl_3) δ 149.21, 136.43, 128.50, 128.09, 126.39, 122.57, 121.27, 52.45, 47.15, 41.20, 40.14, 28.93, 22.44. IR (CDCl_3 , cm^{-1}): 3024, 2968, 2870, 1470, 1387, 1111, 745, 698. HRMS *calcd.* for ($\text{C}_{21}\text{H}_{31}\text{N}_2$) $[\text{M}+\text{H}]^+$: 311.2487, *found* 311.2488.

Note: rotamers were observed in NMR.



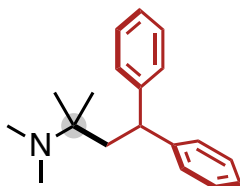
31

***N*-(*tert*-butyl)-*N*-isopropyl-3,3-diphenylpropan-1-amine:** Following the general procedure B, the title compound was obtained in 86% as yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 7.28-7.27 (m, 8H), 7.18-7.17 (m, 2H), 3.87 (t, $J = 7.7$ Hz, 1H), 3.35-3.29 (m, 1H), 2.44-2.40 (m, 2H), 2.21-2.15 (2H), 1.03 (s, 9H), 0.93 (d, $J = 6.4$ Hz, 6H). ^{13}C NMR (101 MHz, CDCl_3) δ 145.47, 128.49, 127.99, 126.12, 55.43, 50.16, 46.97, 41.34, 41.09, 29.13, 22.61. IR (CDCl_3 , cm^{-1}): 3060, 3025, 2935, 1450, 1441, 847, 749, 701. HRMS *calcd.* for ($\text{C}_{22}\text{H}_{32}\text{N}$) $[\text{M}+\text{H}]^+$: 310.2535, *found* 310.2542.



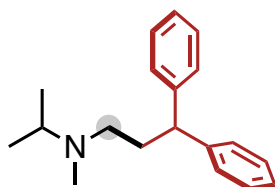
32 (1.8:1)

***N*-isopropyl-*N*,2-dimethyl-4,4-diphenylbutan-2-amine:** Following the general procedure B, the title compound was obtained in 84% as a mixture of yellow oil. Selected peaks for ^1H NMR (400 MHz, CDCl_3) δ 4.20 (t, $J = 6.3$ Hz, 1.78H), 3.92 (t, $J = 7.6$ Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 128.74, 128.67, 127.84, 126.64, 126.17, 49.38, 47.40, 27.64, 24.96, 20.58, 18.86. IR (CDCl_3 , cm^{-1}): 3025, 2964, 2935, 1491, 1444, 841, 749, 701. HRMS *calcd.* for ($\text{C}_{21}\text{H}_{30}\text{N}$) $[\text{M}+\text{H}]^+$: 296.2378, *found* 296.2386.



33

***N,N*,2-trimethyl-4,4-diphenylbutan-2-amine:** Following the general procedure B, the title compound was obtained in 49% as a yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 7.36-7.34 (m, 4H), 7.28-7.24 (m, 4H), 7.16-7.12 (m, 2H), 4.25 (t, $J = 6.2$ Hz, 1H), 2.33 (d, $J = 6.2$ Hz, 2H), 2.27 (s, 6H), 0.93 (s, 6H). ^{13}C NMR (101 MHz, CDCl_3) δ 146.88, 128.59, 127.91, 126.01, 47.05, 44.30, 38.49, 23.62. IR (CDCl_3 , cm^{-1}): 3026, 2975, 2940, 1492, 1261, 1130, 749, 696. HRMS *calcd.* for ($\text{C}_{19}\text{H}_{26}\text{N}$) $[\text{M}+\text{H}]^+$: 268.2065, *found* 268.2070.

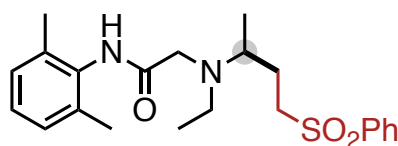


33'

***N*-isopropyl-*N*-methyl-3,3-diphenylpropan-1-amine:** Following the general procedure B, the title compound was obtained in 18% as a yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 7.29-7.25 (m, 8H), 7.19-7.14 (m, 2H), 4.01-3.97 (m, 1H), 3.13-3.06 (m, 1H), 2.58-2.54 (m, 2H), 2.45-2.42 (m, 2H), 2.37 (s, 3H), 1.08 (d, $J = 6.6$ Hz, 6H). ^{13}C NMR (101 MHz, CDCl_3) δ 144.04, 128.70, 127.83, 126.53, 54.73, 51.97, 49.07, 36.18, 31.98, 17.26. IR (CDCl_3 , cm^{-1}): 3026, 2963, 1492, 1451, 1154, 841, 752, 699. HRMS *calcd.* for ($\text{C}_{19}\text{H}_{26}\text{N}$) $[\text{M}+\text{H}]^+$: 268.2065, *found* 268.2065.

General Procedure C for trialkylamine-containing pharmaceuticals: A 8.0 mL disposable borosilicate glass tube with screw cap containing a stirring bar was charged with TPS-SH (20 mol%, 5.8 mg, 0.02 mmol), $\text{Ir}(\text{ppy})_2(\text{dtbbpy})\text{PF}_6$ (1 mol%, 0.9 mg, 0.001 mmol), pharmaceutical (0.3 mmol) and olefin (0.1 mmol, added after solvent if liquid). The tube was transferred to a nitrogen-filled glove-box where the dry Tol (1.0 mL, 0.1 M) was added. Then the reaction was stirred for 1 minute and transferred outside, placing ~10 cm away from a 34 W Blue-Leds and rigorously stirred for 8 h with cooling by fan. After completion of the reaction, the product was directly purified by flash column chromatography in silica gel with $\text{CHCl}_3/\text{MeOH}$.

Note: in case of solubility issue of the drug molecules in Tol, DMA or DMSO (1 mL) could be used as cosolvent.

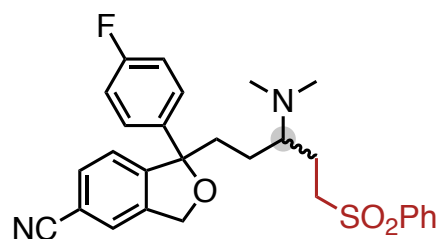


34

***N*-(2,6-dimethylphenyl)-2-(ethyl(4-(phenylsulfonyl)butan-2-yl)amino)acetamide:**

Following the general procedure C, the title compound was obtained in 65% yield after 8 h as colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 8.55 (s, 1H), 7.87 (d, $J = 7.9$ Hz, 2H), 7.66 (t, $J = 7.4$ Hz, 1H), 7.55 (t, $J = 7.7$ Hz, 2H), 7.13-7.06 (m, 3H), 3.24-3.10 (m, 4H), 3.00-2.95 (m, 1H), 2.65-2.59 (m, 2H), 2.19 (s, 6H), 2.04-1.94 (m, 1H), 1.81-1.72 (m, 1H), 1.14 (t, $J = 7.1$ Hz, 1H), 1.05 (d, $J = 6.5$ Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 170.06, 139.06, 135.22, 134.02, 133.76, 129.55, 128.44, 128.04, 127.44, 54.89, 54.28, 54.04, 45.89, 26.76, 18.76, 14.92, 14.25. IR

(CDCl₃, cm⁻¹): 3300, 3062, 2967, 1671, 1491, 1303, 1086, 731. HRMS *calcd.* for (C₂₂H₃₁N₂O₃S) [M+H]⁺: 403.2055, *found* 403.2068.

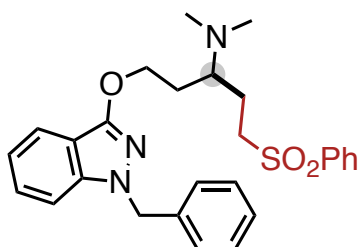


35 (~ dr. 1:1)

1-(3-(dimethylamino)-5-(phenylsulfonyl)pentyl)-1-(4-fluorophenyl)-1,3-

dihydroisobenzofuran-5-carbonitrile: Following the general procedure C, the title compound was obtained in 55% yield (~ dr. 1:1) after 8 h as colorless oil. ¹H NMR (400 MHz, CDCl₃) δ 7.89 (d, *J* = 7.7 Hz, 1H), 7.66-7.54 (m, 4H), 7.50 (s, 1H), 7.41-7.36 (m, 3H), 7.01 (t, *J* = 8.6 Hz, 1H), 5.19-5.10 (m, 2H), 3.20-2.99 (m, 2H), 2.35 (br, 1H), 2.22-2.05 (m, 2H), 2.05 (s, 6H), 1.81-1.71 (m, 2H), 1.52-1.33 (m, 1H), 1.18-1.00 (m, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 163.45, 161.00, 149.50, 149.46, 140.40, 140.26, 139.69, 139.67, 139.33, 133.76, 132.10, 132.05, 129.41, 128.04, 128.03, 126.87, 126.84, 126.79, 126.77, 125.42, 122.80, 122.77, 118.69, 115.69, 115.48, 112.04, 91.21, 91.21, 71.36, 71.33, 62.76, 62.70, 54.05, 40.13, 40.11, 38.60, 22.79, 22.71, 22.65. ¹⁹F NMR (376 MHz, CDCl₃) δ -115.12. IR (CDCl₃, cm⁻¹): 3064, 2937, 2826, 2228, 1506, 1303, 1032, 732. HRMS *calcd.* for (C₂₈H₃₀N₂O₃FS) [M+H]⁺: 493.1961, *found* 493.1969.

Note: less than 10% of minor isomer (impure) was observed.



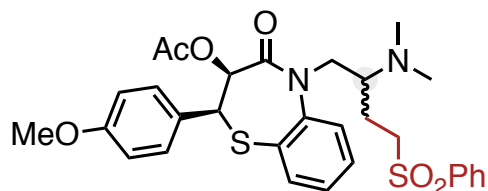
36

1-((1-benzyl-1H-indazol-3-yl)oxy)-N,N-dimethyl-5-(phenylsulfonyl)pentan-3-amine:

Following the general procedure C, the title compound was obtained in 63% yield after 8 h as colorless oil. ¹H NMR (400 MHz, CDCl₃) δ 7.90-7.88 (m, 2H), 7.61-7.56 (m, 2H), 7.50-7.46 (m, 2H), 7.33-7.23 (m, 4H), 7.19-7.16 (m, 3H), 7.03 (t, *J* = 7.8 Hz, 1H), 5.38 (s, 2H), 4.37 (tt, *J* = 10.4, 5.3 Hz, 2H), 3.39-3.32 (m, 1H), 3.19-3.12 (m, 1H), 2.68 (br, 1H), 2.17 (s, 6H), 2.15-2.08 (m, 1H), 1.98-1.86 (m, 2H), 1.62 (dq, *J* = 14.1, 6.4 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 155.82, 141.71, 139.59, 137.57, 133.61, 129.32, 128.71, 128.09, 127.64, 127.54, 127.16,

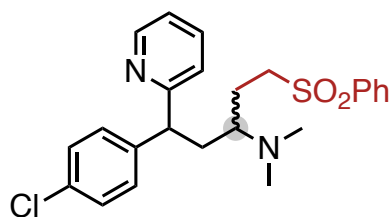
120.10, 119.32, 113.14, 108.99, 66.95, 59.79, 53.98, 52.48, 40.05, 27.54, 24.13. IR (CDCl₃, cm⁻¹): 3061, 2937, 2780, 1528, 1444, 1303, 1086, 742. HRMS *calcd.* for (C₂₇H₃₂N₃O₃S) [M+H]⁺: 478.2164, *found* 478.2166.

Note: less than 10% of minor isomer (impure) was observed.



37 (~dr. 1.2:1)

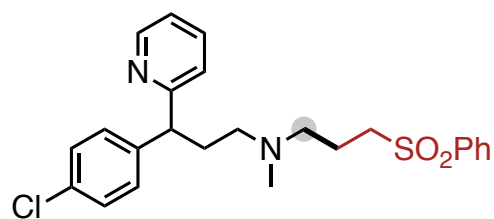
(2R,3S)-5-(2-(dimethylamino)-4-(phenylsulfonyl)butyl)-2-(4-methoxyphenyl)-4-oxo-2,3,4,5-tetrahydrobenzo[b][1,4]thiazepin-3-yl acetate: Following the general procedure C, the title compound was obtained in 76% yield (~dr. 1.2:1) after 8 h as colorless oil. ¹H NMR (400 MHz, CDCl₃) δ 7.88 (d, *J* = 7.8 Hz, 1H), 7.75 (d, *J* = 7.6 Hz, 1H), 7.71-7.56 (m, 2H), 7.56-7.24 (m, 7H), 6.94 (d, *J* = 8.6 Hz, 1H), 6.87 (d, *J* = 8.6 Hz, 1H), [5.13 (d, *J* = 7.7 Hz, 0.55H), 5.08 (d, *J* = 7.5 Hz, 0.45H)], [4.99 (d, *J* = 7.8 Hz, 0.55H), 4.96 (d, *J* = 7.5 Hz, 0.45H)], 4.47-4.41 (m, 1H), [3.83 (s, 1.58H), 3.81 (s, 1.29H)], 3.60-2.96 (m, 4H), 2.52-2.19 (m, 4H), 2.06-2.04 (m, 4H), 1.88-1.87 (m, 3H), 1.75-1.43 (m, 1H). Major isomer: ¹³C NMR (126 MHz, CDCl₃) δ 170.03, 159.96, 139.21, 135.95, 133.58, 131.43, 130.91, 129.37, 128.98, 128.31, 128.13, 127.46, 126.45, 124.85, 123.68, 114.07, 71.32, 60.89, 55.41, 54.63, 53.74, 46.18, 39.98, 22.37, 20.60. IR (CDCl₃, cm⁻¹): 3063, 2937, 2833, 1744, 1676, 1511, 1147, 731. HRMS *calcd.* for (C₃₀H₃₅N₂O₆S₂) [M+H]⁺: 583.1937, *found* 583.1946.



38 (~dr. 1:1)

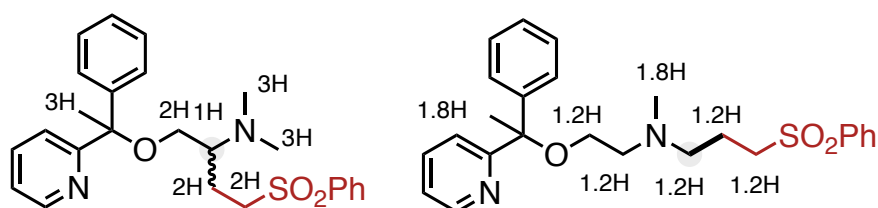
1-(4-chlorophenyl)-N,N-dimethyl-5-(phenylsulfonyl)-1-(pyridin-2-yl)pentan-3-amine: Following the general procedure C, the title compound was obtained in 59% yield (~dr. 1:1) after 8 h as colorless oil. ¹H NMR (400 MHz, CDCl₃) δ 8.58-8.54 (m, 1H), 7.90-7.87 (m, 2H), 7.66 (t, *J* = 7.4 Hz, 1H), 7.56 (t, *J* = 7.7 Hz, 3H), 7.28-7.23 (m, 4H), 7.13-7.09 (m, 2H), 4.16-4.09 (m, 1H), 3.23-3.02 (m, 2H), 2.51-2.18 (m, 2H), 2.12 (s, 3H), 2.10 (s, 3H), 1.93-1.76 (m, 3H). ¹³C NMR (101 MHz, CDCl₃) δ (162.79, 162.64), (149.53, 149.49), (142.42, 141.88), (139.64, 139.57), 136.62, (133.68, 133.63), (132.49, 132.40), (129.48, 129.45), (129.35, 129.33), (128.81, 128.75), 128.06, 123.42, 121.69, (60.12, 59.95), (54.14, 54.02), (49.66,

49.46), 39.88, (34.49, 33.74), (22.57, 22.39). IR (CDCl₃, cm⁻¹): 3063, 2934, 2824, 1587, 1470, 1302, 1086, 731. HRMS *calcd.* for (C₂₄H₂₈N₂O₂SO₂) [M+H]⁺: 443.1560, *found* 443.1560.



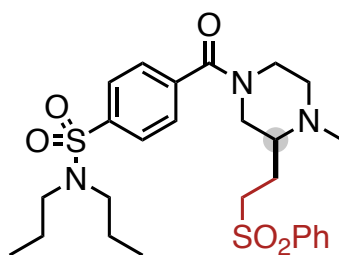
38'

3-(4-chlorophenyl)-N-methyl-N-(3-(phenylsulfonyl)propyl)-3-(pyridin-2-yl)propan-1-amine: Following the general procedure C, the title compound was obtained in 16% yield after 8 h as colorless oil. ¹H NMR (400 MHz, CDCl₃) δ 8.57 (d, *J* = 4.3 Hz, 1H), 7.92 (d, *J* = 7.6 Hz, 2H), 7.67 (t, *J* = 7.4 Hz, 1H), 7.60-7.55 (m, 3H), 7.28-7.24 (m, 4H), 7.13-7.10 (m, 2H), 4.08 (t, *J* = 7.5 Hz, 1H), 3.16-3.12 (m, 2H), 2.45-2.36 (m, 3H), 2.29-2.21 (m, 2H), 2.17-2.09 (m, 4H), 1.88-1.79 (m, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 163.01, 149.55, 142.20, 139.43, 136.67, 133.76, 132.40, 129.49, 129.41, 128.78, 128.16, 123.01, 121.67, 55.61, 54.26, 50.54, 41.64, 32.44, 20.70. IR (CDCl₃, cm⁻¹): 3062, 2949, 2797, 1587, 1305, 1087, 822, 750. HRMS *calcd.* for (C₂₄H₂₈N₂O₂SO₂) [M+H]⁺: 443.1560, *found* 443.1562.



39 (~dr. 1:1, ~rr. 1.7:1)

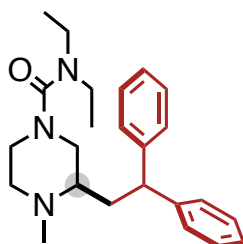
Following the general procedure C, the title compound was obtained in 73% yield as a yellow oil mixture after 8h. ¹H NMR (400 MHz, CDCl₃) δ 8.52-7.08 (m, 22.4H), 3.41-3.16 (m, 6.4H), 2.69-2.64 (m, 1H), 2.60 (t, *J* = 5.9 Hz, 1.2H), 2.48 (t, *J* = 6.6 Hz, 1.2H), 2.23 (s, 3H), 2.22 (3H), 2.18 (s, 1.8H), 2.01-1.85 (m, 8H). Selected peaks: ¹³C NMR (101 MHz, CDCl₃) δ 165.05, 148.54, 136.52, 133.62, 129.32, 128.16, 126.45, 121.86, 121.02, 82.41, 62.28, 57.39, 54.22, 41.22, 24.06, 20.85. IR (CDCl₃, cm⁻¹): 3058, 2934, 2783, 1446, 1303, 1085, 789, 748. HRMS *calcd.* for (C₂₅H₃₁N₂O₃S) [M+H]⁺: 439.2055, *found* 439.2057.



40
78

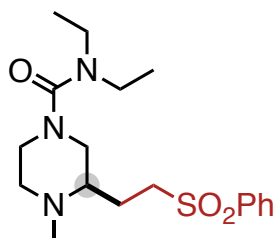
4-(4-methyl-3-(2-(phenylsulfonyl)ethyl)piperazine-1-carbonyl)-N,N-

dipropylbenzenesulfonamide: Following the general procedure C, the title compound was obtained in 77% yield after 8 h as colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 7.95-7.78 (m, 4H), 7.68-7.64 (m, 1H), 7.59-7.55 (m, 2H), 7.50-7.42 (br, 2H), 4.36-4.11 (br, 1H), 3.42-2.61 (m, 10 H), 2.40-2.15 (m, 5 H), 2.05-1.73 (br, 2H), 1.55 (h, $J = 7.4$ Hz, 4H), 0.86 (t, $J = 7.4$ Hz, 6H). ^{13}C NMR (101 MHz, CDCl_3) δ 168.77, 141.67, 139.18, 139.08, 134.00, 129.55, 128.08, 127.73, 127.49, 59.48, 54.22, 51.69, 50.24, 47.16, 44.91, 41.99, 22.19, 21.80, 11.26. IR (CDCl_3 , cm^{-1}): 3064, 2965, 1630, 1443, 1147, 1086, 913, 726. HRMS *calcd.* for ($\text{C}_{26}\text{H}_{38}\text{N}_3\text{O}_5\text{S}_2$) $[\text{M}+\text{H}]^+$: 536.2253, *found* 536.2262.



41

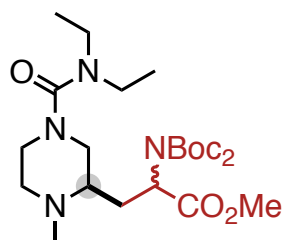
3-(2,2-diphenylethyl)-N,N-diethyl-4-methylpiperazine-1-carboxamide: Following the general procedure C, 5 mol% of TPS-SH and 50 mol% of 2-*tert*-butyl-1,1,3,3-tetramethylguanidine (Barton's base) was used instead of 10 mol% of TPS-SH, the title compound was obtained in 45% yield after 8 h as colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 7.31-7.14(m, 10H), 4.02 (dd, $J = 10.0, 5.7$ Hz, 1H), 3.44-3.35 (m, 2H), 3.14-3.00 (m, 5H), 2.82-2.73 (m, 2H), 2.52 (ddd, $J = 13.5, 10.1, 2.9$ Hz, 1H), 2.30 (s, 3H), 2.24 (td, $J = 11.5, 3.1$ Hz, 1H), 2.07-2.03 (m, 1H), 1.95 (ddd, $J = 14.1, 8.4, 5.7$ Hz, 1H), 1.05 (t, $J = 7.1$ Hz, 6H). ^{13}C NMR (101 MHz, CDCl_3) δ 164.40, (145.26, 143.86), (128.76, 128.68), (128.11, 127.78), (126.61, 126.41), 60.24, 54.44, 51.32, 48.45, 46.40, 42.52, 41.86, 35.55, 13.35. IR (CDCl_3 , cm^{-1}): 3065, 2968, 2794, 1640, 1451, 1416, 1261, 701. HRMS *calcd.* for ($\text{C}_{24}\text{H}_{34}\text{N}_3\text{O}$) $[\text{M}+\text{H}]^+$: 380.2702, *found* 380.2710.



42

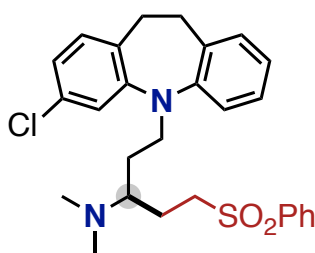
N,N-diethyl-4-methyl-3-(2-(phenylsulfonyl)ethyl)piperazine-1-carboxamide: Following the general procedure C, the title compound was obtained in 82% yield after 8 h as colorless

oil. ^1H NMR (400 MHz, CDCl_3) δ 7.90 (d, $J = 8.0$ Hz, 2H), 7.65 (t, $J = 6.9$ Hz, 1H), 7.56 (t, $J = 7.7$ Hz, 2H), 3.37-3.23 (m, 3H), 3.16 (q, $J = 7.1$ Hz, 4H), 3.11-3.02 (m, 1H), 2.93 (t, $J = 11.6$ Hz, 1H), 2.71 (d, $J = 11.7$ Hz, 1H), 2.61 (t, $J = 11.3$ Hz, 1H), 2.39-2.24 (m, 2H), 2.19 (s, 3H), 2.05-1.87 (m, 2H), 1.08 (t, $J = 7.1$ Hz, 6H). ^{13}C NMR (101 MHz, CDCl_3) δ 164.31, 139.21, 133.89, 129.46, 128.12, 59.71, 54.73, 51.79, 49.86, 47.22, 42.23, 41.87, 22.63, 13.29. IR (CDCl_3 , cm^{-1}): 3062, 2969, 2797, 1634, 1419, 1262, 1086, 735. HRMS *calcd.* for ($\text{C}_{18}\text{H}_{30}\text{N}_3\text{O}_3\text{S}$) $[\text{M}+\text{H}]^+$: 368.2008, *found* 368.2030.



43

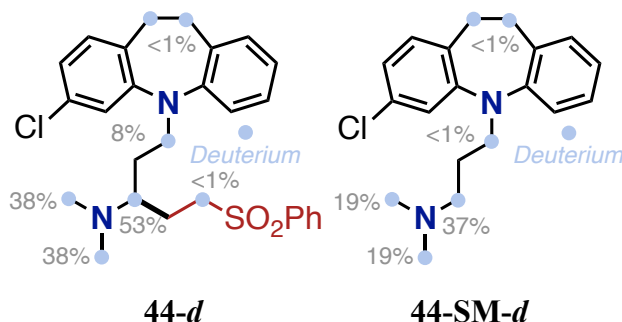
methyl 2-(bis(*tert*-butoxycarbonyl)amino)-3-(4-(diethylcarbamoyl)-1-methylpiperazin-2-yl)propanoate: Following the general procedure C, the title compound was obtained in 73% yield (~dr. 1.4:1) after 8 h as colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 5.00-4.96 (m, 1H), 3.70 (s, 3H), 3.45-2.57 (m, 10H), 2.34-2.15 (m, 6H), 1.48 (s, 18H), 1.10 (t, $J = 7.1$ Hz, 3H), 1.09 (t, $J = 7.1$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ (171.46, 171.35), 164.49, (152.24, 152.11), (83.42, 83.35), (59.78, 59.36), (55.87, 55.80), (54.74, 53.97), 52.42, (51.42, 51.07), (46.55, 46.27), (42.67, 42.42), 41.91, (31.95, 29.19), 28.13, 13.31. IR (CDCl_3 , cm^{-1}): 2977, 2934, 1793, 1745, 1699, 1645, 1366, 777. HRMS *calcd.* for ($\text{C}_{24}\text{H}_{45}\text{N}_4\text{O}_7$) $[\text{M}+\text{H}]^+$: 501.3288, *found* 501.3291.



44

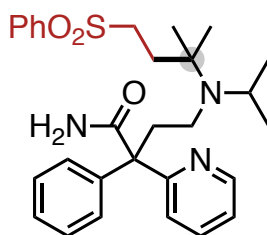
1-(3-chloro-10,11-dihydro-5H-dibenzo[*b,f*]azepin-5-yl)-*N,N*-dimethyl-5-(phenylsulfonyl)pentan-3-amine: Following the general procedure C with ethyl acetate and hexane as column eluent, the title compound was obtained in 62% yield after 8 h as colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 7.85 (d, $J = 8.0$ Hz, 2H), 7.62 (t, $J = 7.4$ Hz, 1H), 7.52 (t, $J = 7.7$ Hz, 2H), 7.17-7.09 (m, 2H), 7.03-6.94 (m, 4H), 6.87-6.85 (m, 1H), 3.75-3.72 (m, 1H), 3.59 (dt, $J = 13.5, 7.0$ Hz, 1H), 3.20-2.99 (m, 6H), 2.51 (br, 1H), 2.03 (s, 6H), 1.82-1.71 (m,

3H), 1.30-1.24 (m, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 148.96, 147.61, 139.33, 135.28, 133.73, 131.68, 131.56, 131.46, 129.68, 129.36, 128.07, 126.74, 123.66, 122.33, 120.52, 119.76, 60.19, 53.78, 48.04, 39.94, 32.21, 31.54, 26.20, 23.11. IR (CDCl_3 , cm^{-1}): 3062, 2929, 2826, 1585, 1483, 1303, 1086, 731. HRMS *calcd.* for ($\text{C}_{27}\text{H}_{32}\text{N}_2\text{O}_2\text{SCl}$) $[\text{M}+\text{H}]^+$: 483.1873, *found* 483.1879.



Following the general procedure C in presence of D_2O (50 eq.), compound **33-d** was obtained in 60% yield after 8 h as colorless oil, the remaining unreactive starting material **33-SM-d** (2.2 eq.) was recovered.

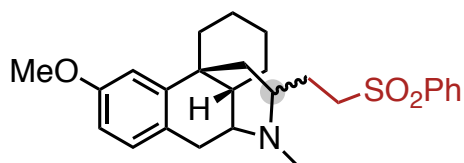
Note: see below H-NMR spectrums for details.



45

4-(isopropyl(2-methyl-4-(phenylsulfonyl)butan-2-yl)amino)-2-phenyl-2-(pyridin-2-yl)butanamide: Following the general procedure C, the title compound was obtained in 71% yield after 8 h as yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 8.69 (br, 1H), 8.55-8.53 (m, 1H), 7.92-7.90 (m, 2H), 7.66-7.60 (m, 2H), 7.58-7.54 (m, 2H), 7.31-7.16 (m, 7H), 5.80 (br, 1H), 3.24-3.20 (m, 2H), 2.90 (p, $J = 6.5$ Hz, 1H), 2.68-2.62 (m, 1H), 2.42-2.30 (m, 2H), 2.25-2.19 (m, 1H), 1.70 (dd, $J = 11.6, 4.7$ Hz, 1H), 0.92 (s, 3H), 0.88 (s, 3H), 0.78 (d, $J = 6.5$ Hz, 3H), 0.74 (d, $J = 6.5$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 175.64, 163.44, 147.26, 144.44, 139.71, 136.95, 133.61, 129.35, 128.37, 128.22, 128.10, 124.50, 121.82, 60.70, 57.36, 52.61, 46.76, 42.66, 37.91, 34.01, 26.60, 26.40, 22.23. IR (CDCl_3 , cm^{-1}): 3274, 3060, 2970, 1675, 1586, 1290, 1145, 730. HRMS *calcd.* for ($\text{C}_{29}\text{H}_{38}\text{N}_3\text{O}_3\text{S}$) $[\text{M}+\text{H}]^+$: 508.2634, *found* 508.2652.

Note: single isomer was obtained due to the β -cleavage of secondary α -amino radical. The by-product diaryl acetamide was isolated as an evidence.



46 (~dr. 5.5:1)

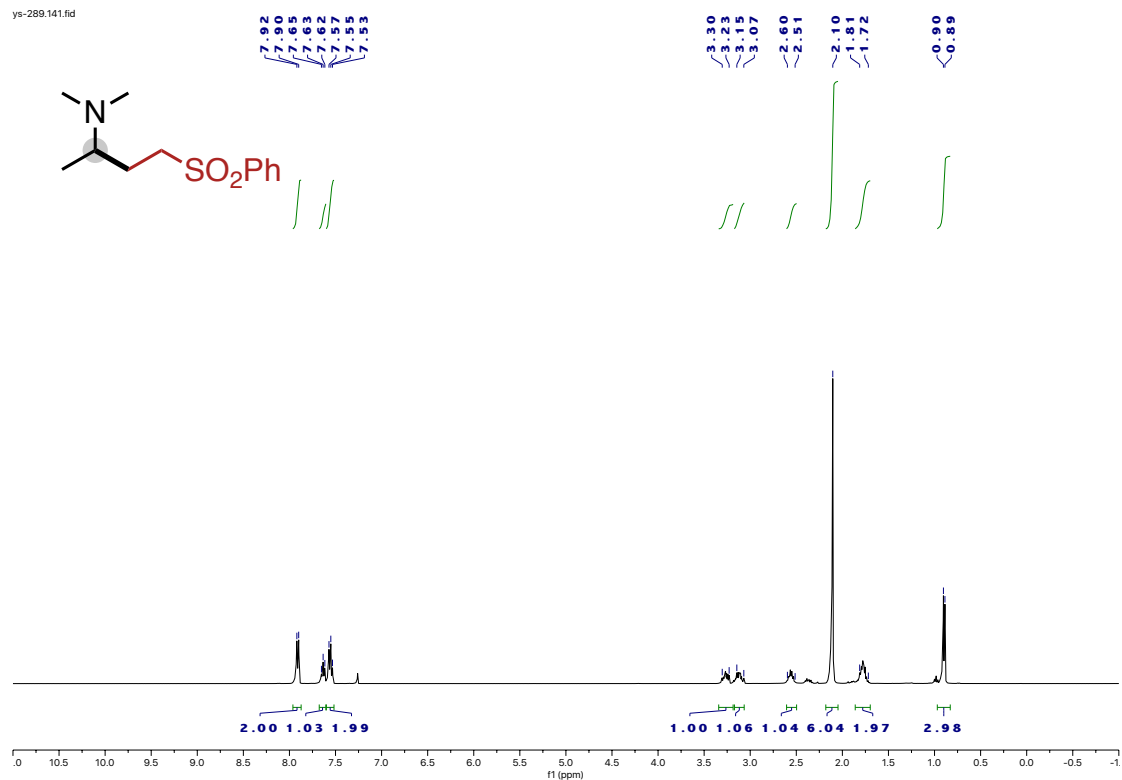
(4b*S*,8a*S*)-3-methoxy-11-methyl-12-(2-(phenylsulfonyl)ethyl)-6,7,8,8a,9,10-hexahydro-5*H*-9,4*b*-(epiminoethano)phenanthrene: Following the general procedure C, the title compound was obtained in 45% yield (~dr. 5.5:1) after 8 h as colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 7.93-7.86 (m, 2H), 7.65-7.61 (m, 1H), 7.57-7.52 (m, 2H), 6.99 (d, $J = 8.3$ Hz, 1H), 6.74 (d, $J = 2.6$ Hz, 1H), 6.69 (dd, $J = 8.3, 2.5$ Hz, 1H), 3.77 (s, 3H), 3.26-2.16 (m, 10 H), 1.85-1.03 (m, 12H). Major isomer: ^{13}C NMR (101 MHz, CDCl_3) δ 158.34, 141.66, 139.29, 133.59, 129.28, 129.23, 128.74, 128.01, 111.09, 110.93, 60.22, 55.20, 52.81, 51.38, 46.84, 44.76, 39.37, 38.04, 36.59, 26.46, 26.36, 24.68, 21.98. IR (CDCl_3 , cm^{-1}): 3061, 2926, 2854, 1497, 1303, 1238, 1145, 730. HRMS *calcd.* For ($\text{C}_{26}\text{H}_{34}\text{NO}_3\text{S}$) $[\text{M}+\text{H}]^+$: 440.2260, *found* 440.2250.

VI. References

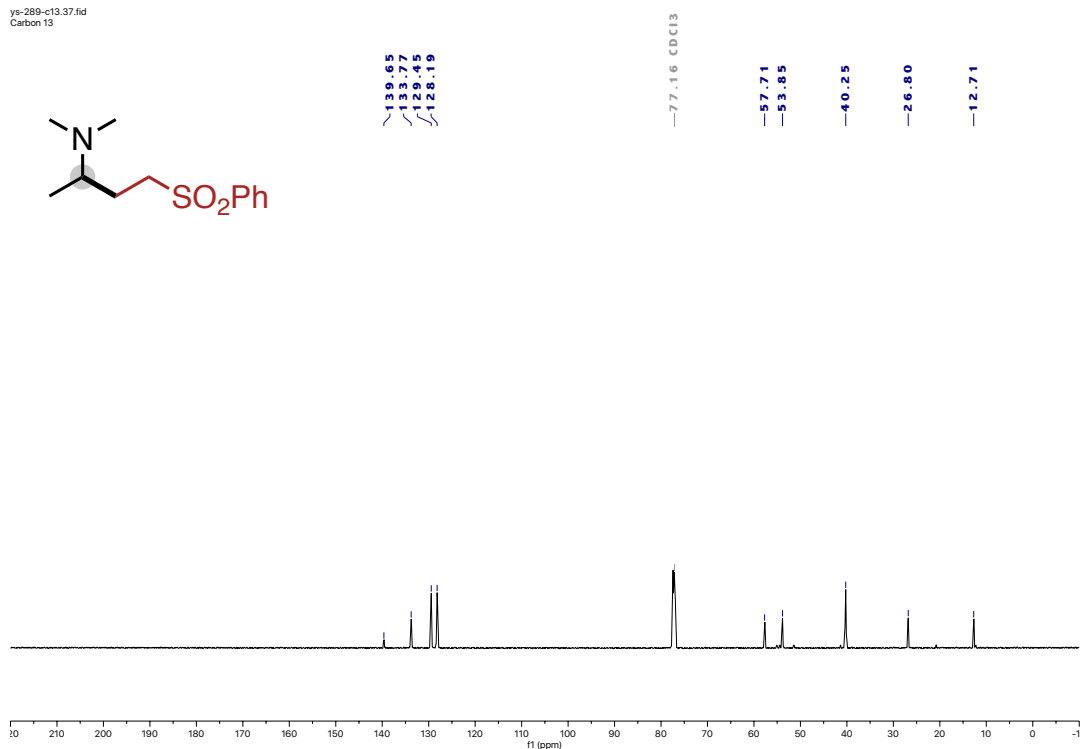
1. Cismesia, M. A.; Yoon, T. P. Characterizing chain processes in visible light photoredox catalysis. *Chem. Sci.*, **2015**, *6*, 5426-5434
2. Zhou, R., Goh, Y. Y., Liu, H., Tao, H., Li, L., Wu, J. Visible-light-mediated metal-free hydrosilylation of alkenes through selective hydrogen atom transfer for Si-H activation. *Angew. Chem. Int. Ed.* **56**, 16621-16625 (2017).
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4. Legault, C. Y. CYLview, Version 1.0b. Université de Sherbrooke. (2009); <http://www.cylview.org>.

VII. ^1H , ^{13}C and ^{19}F NMR spectra

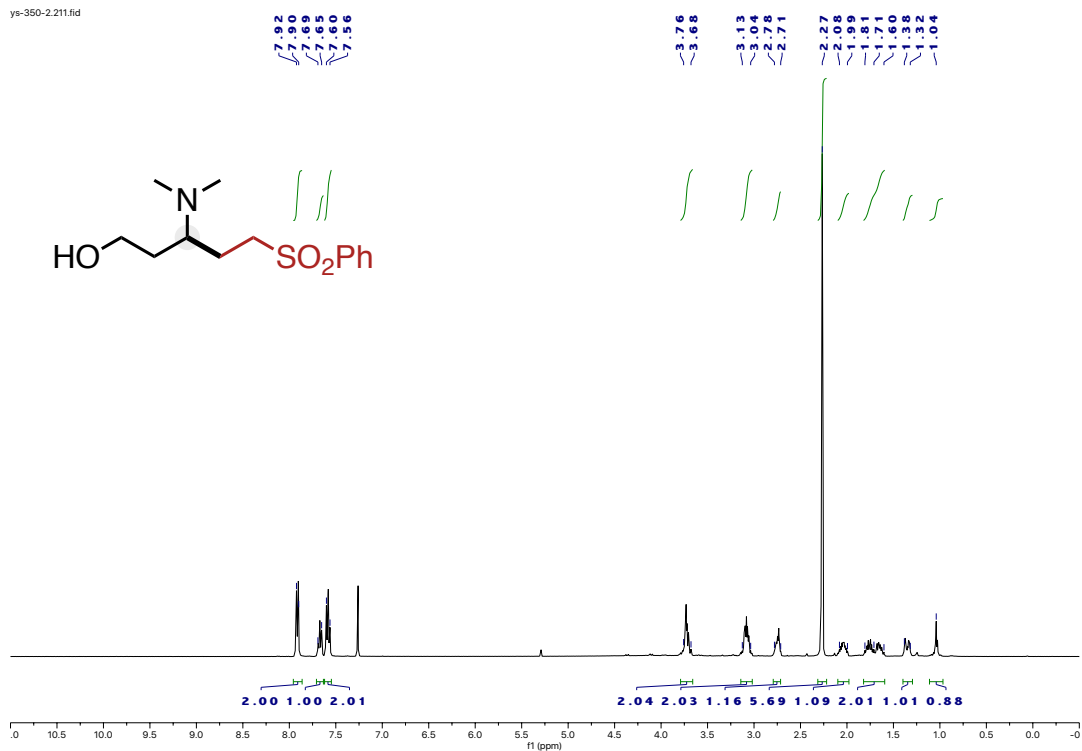
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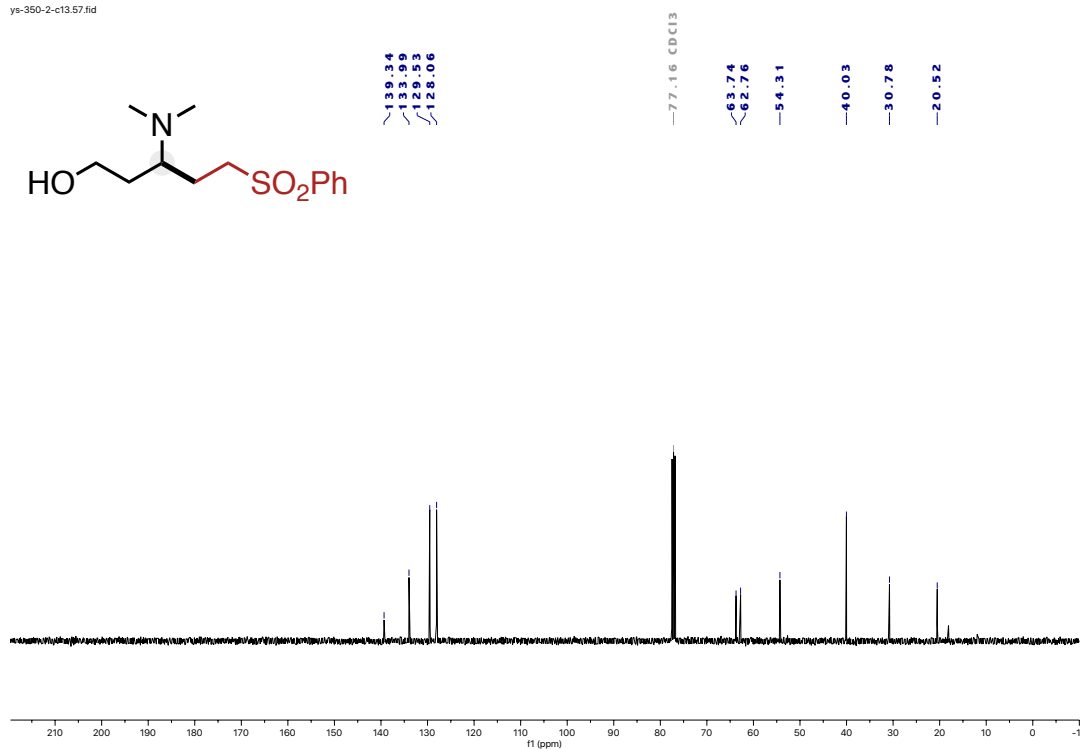
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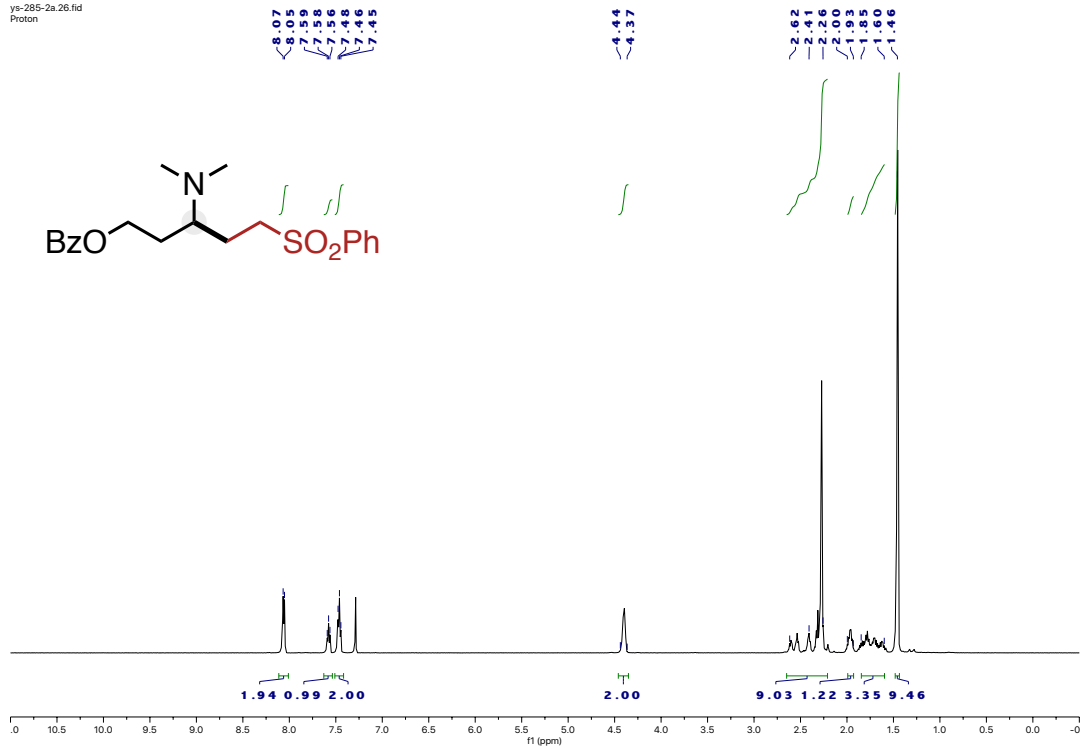
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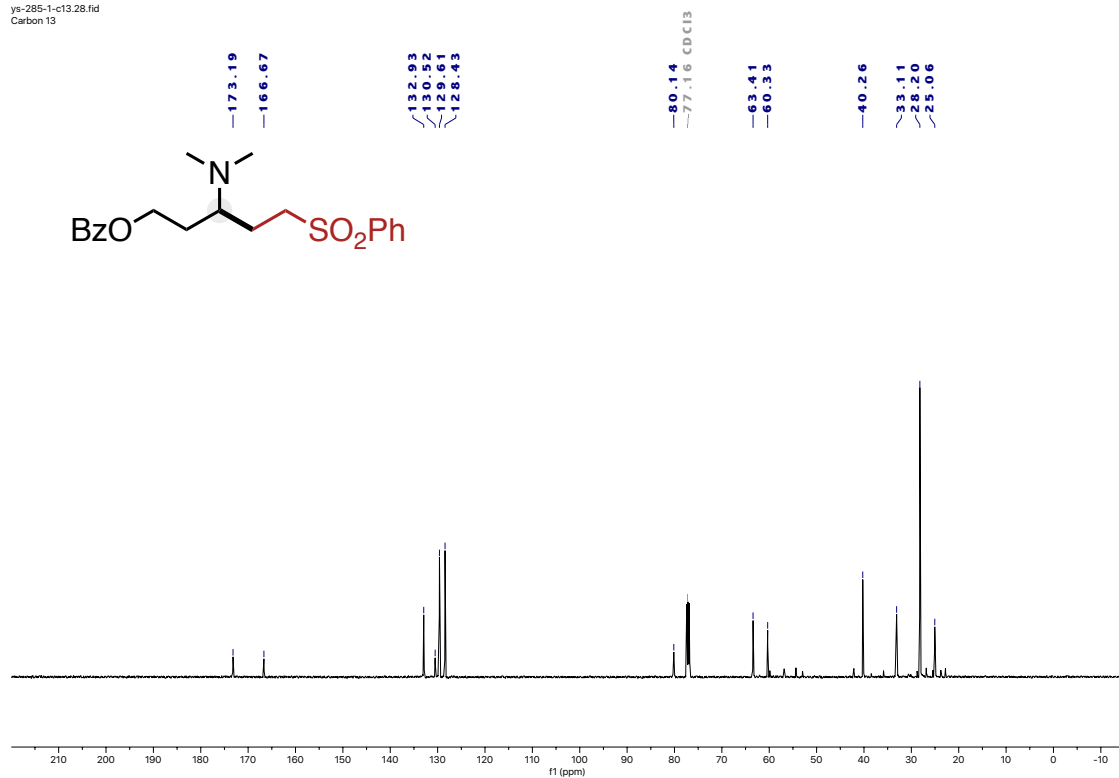
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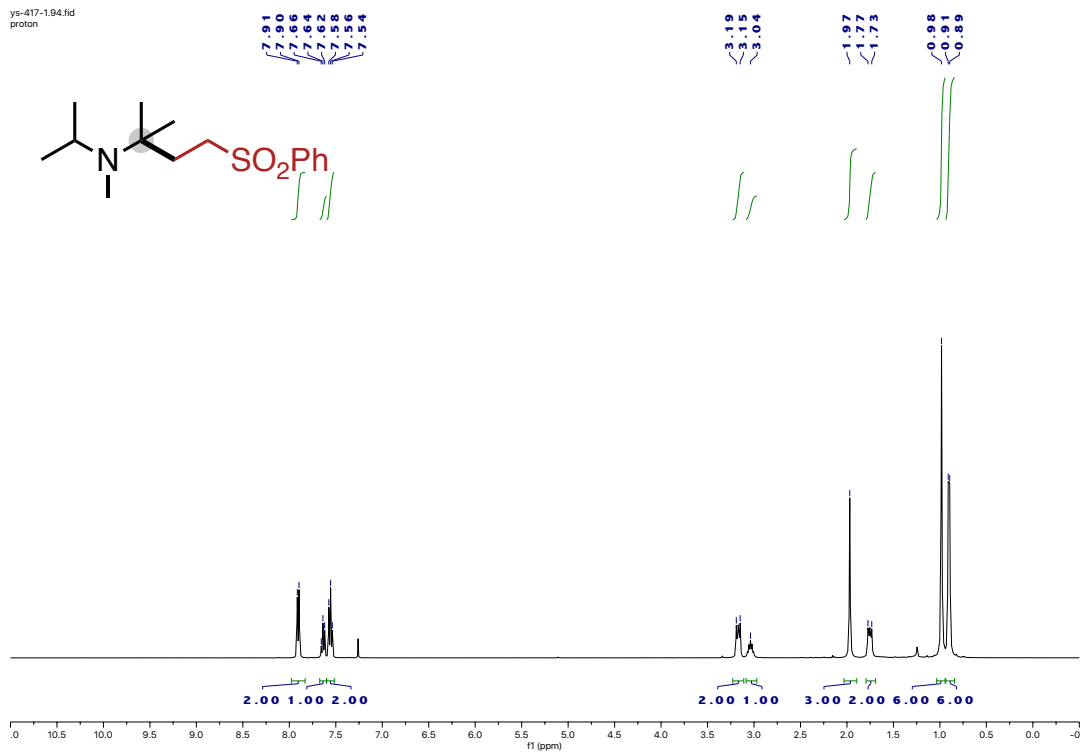
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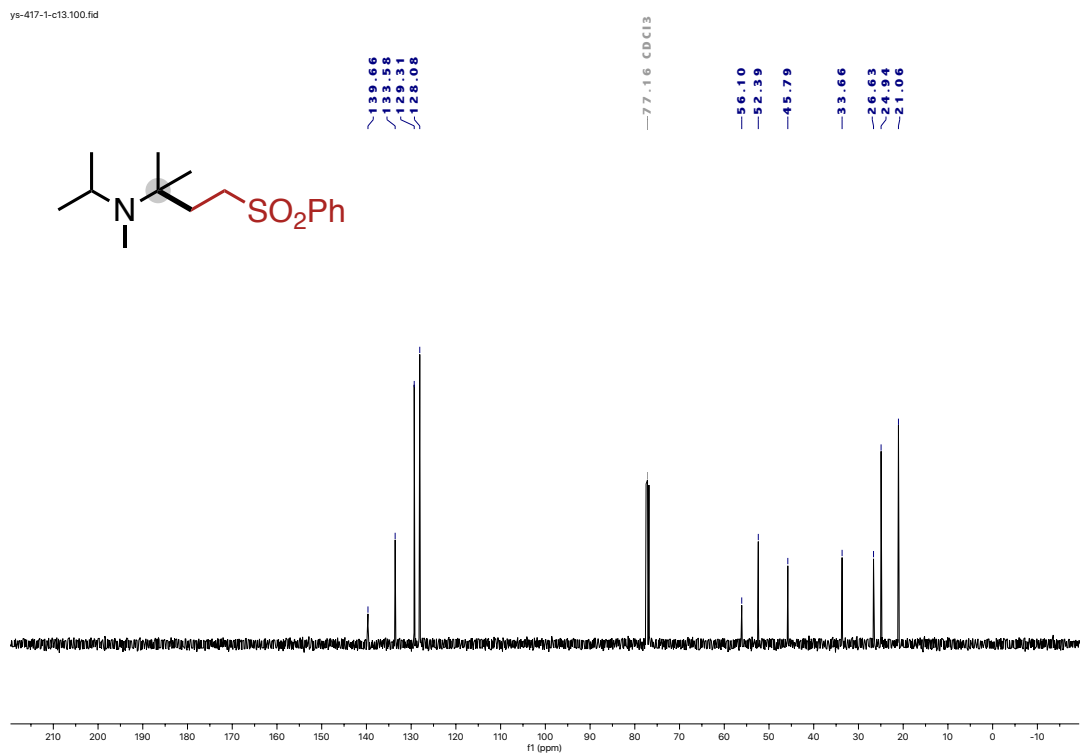
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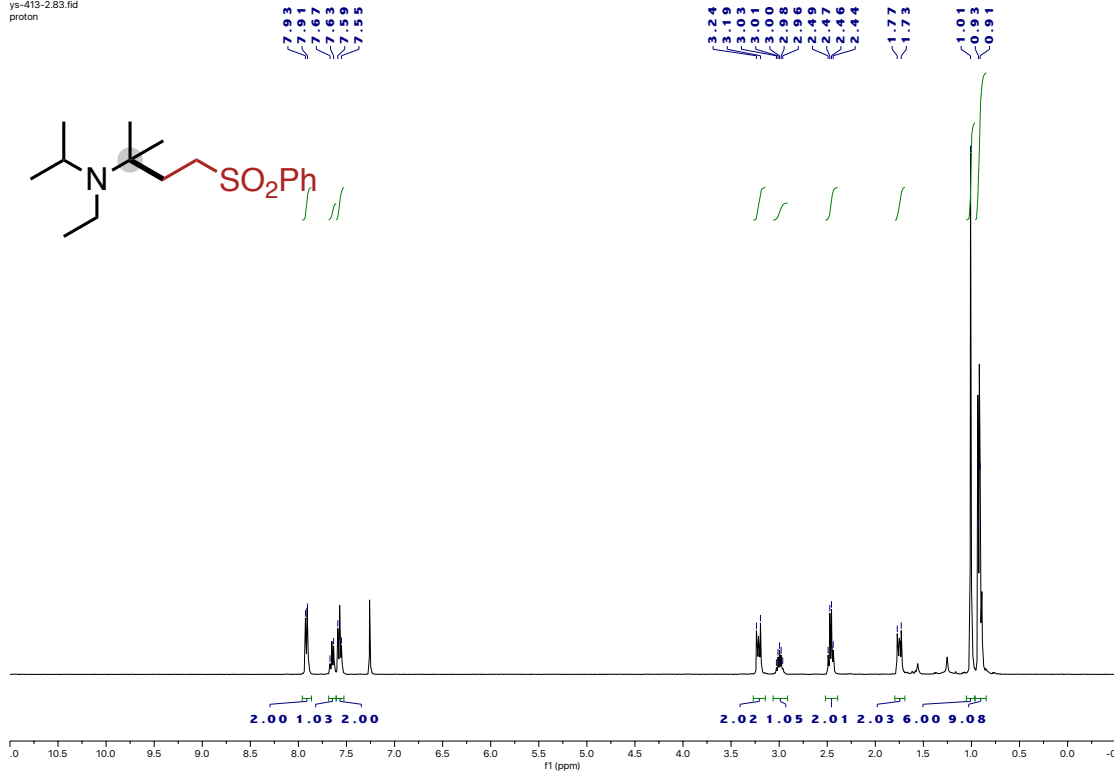
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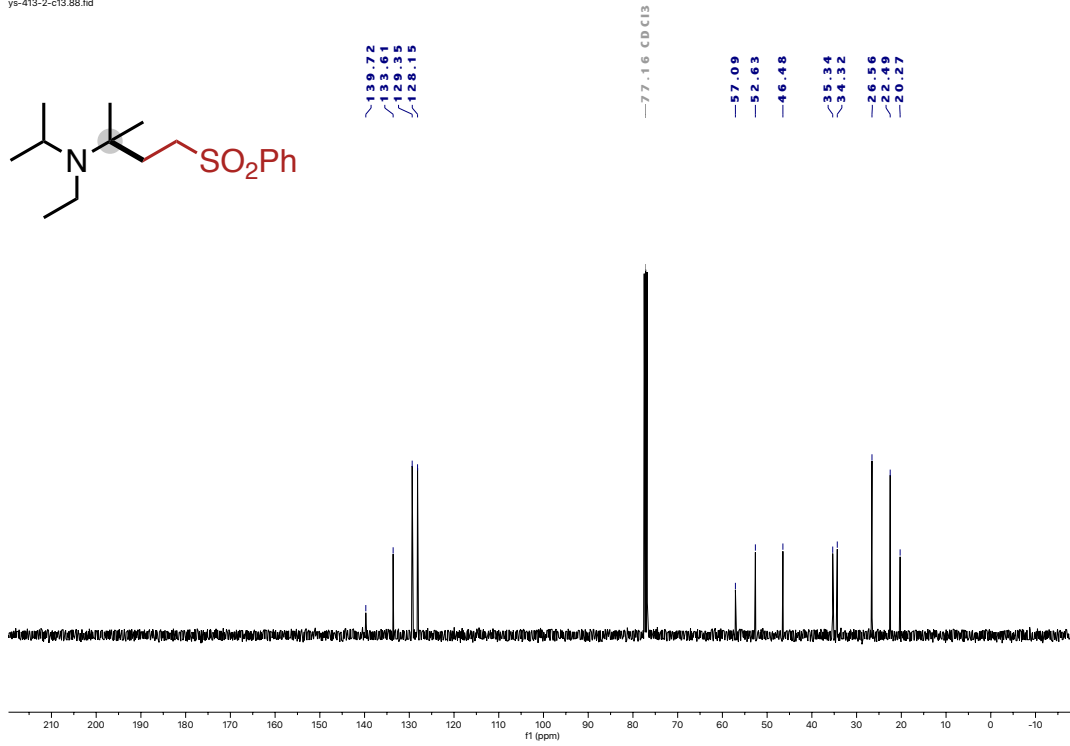
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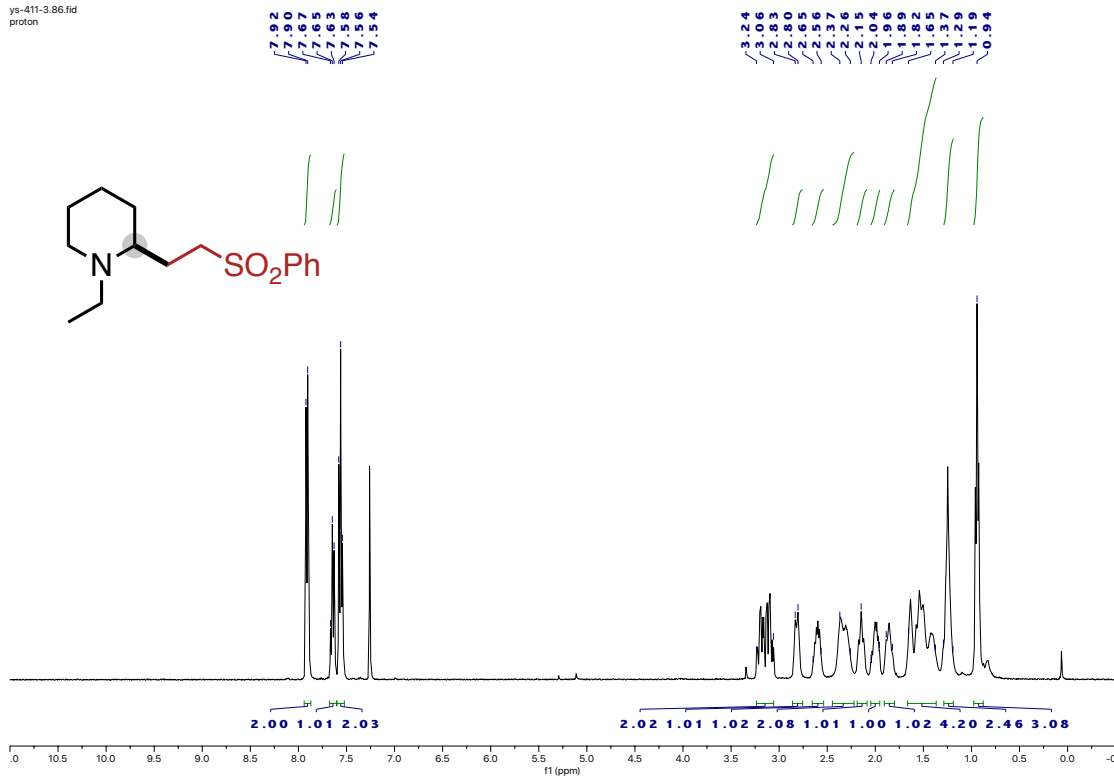
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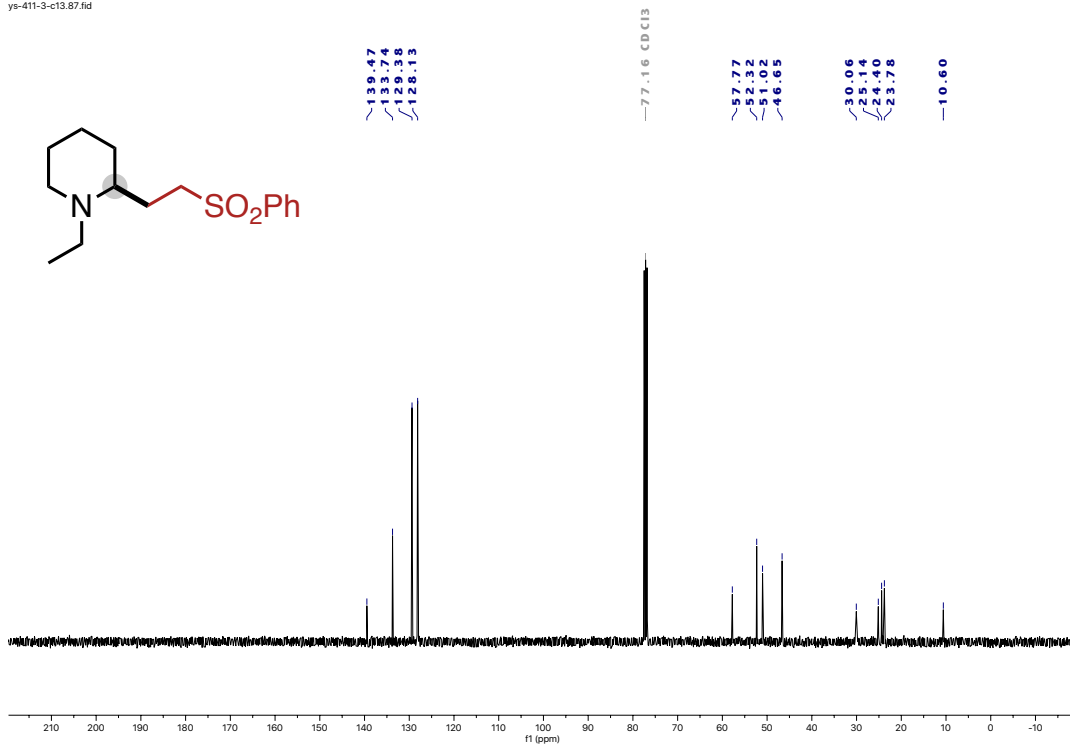
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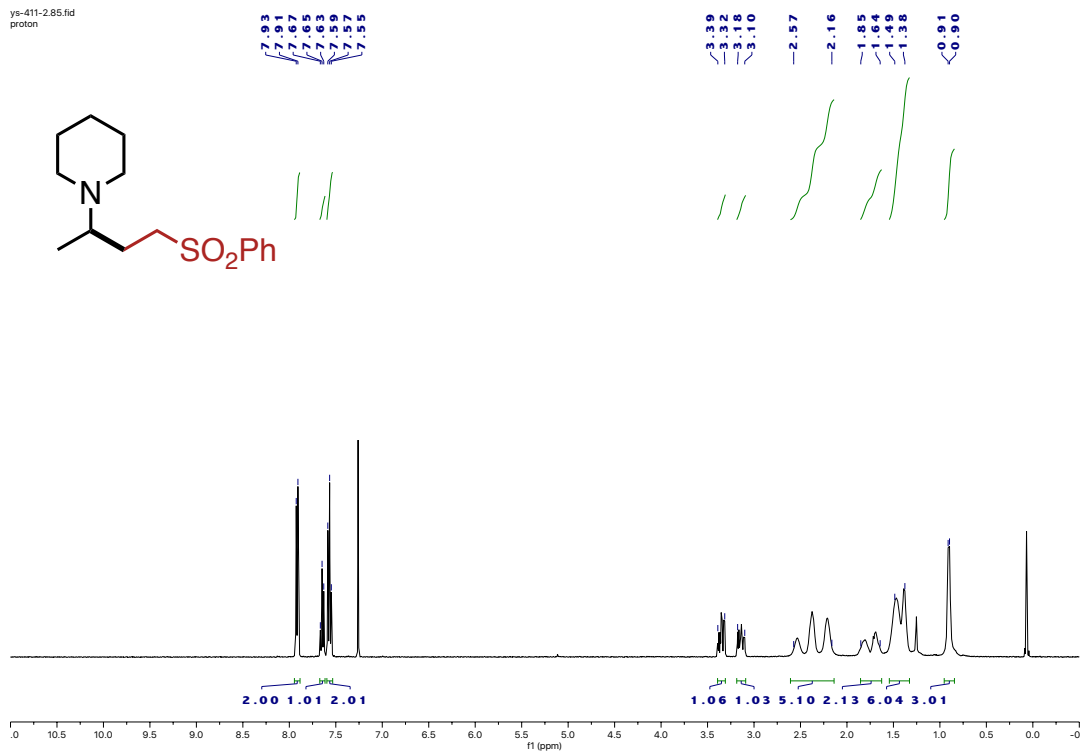
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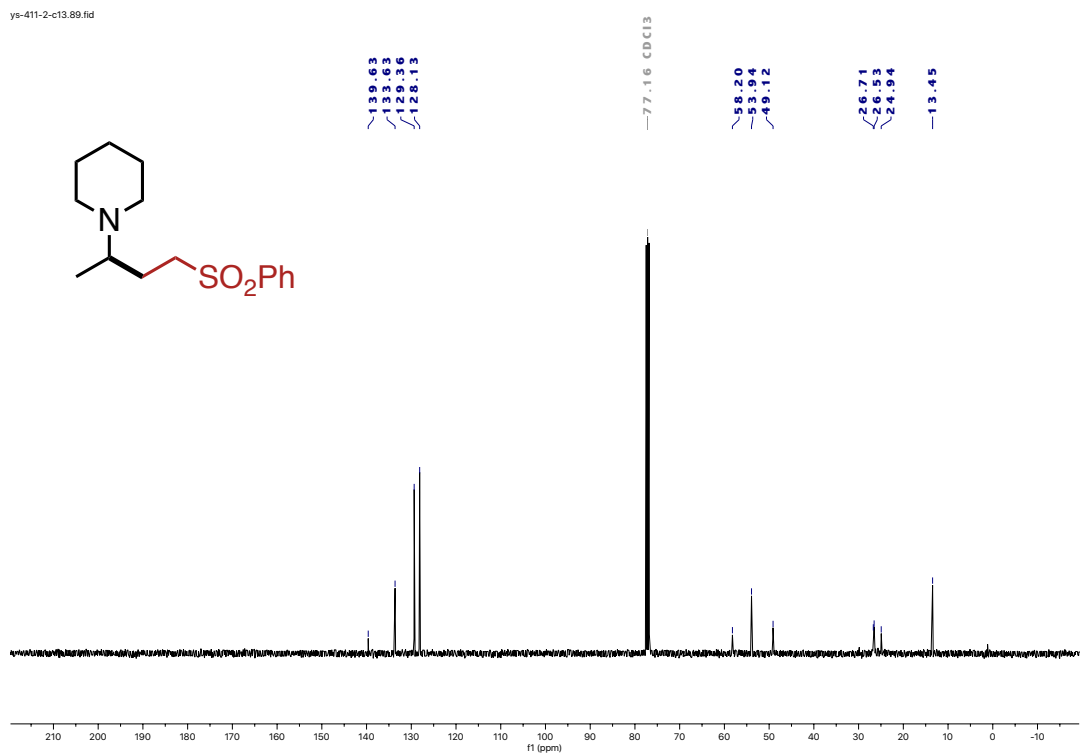
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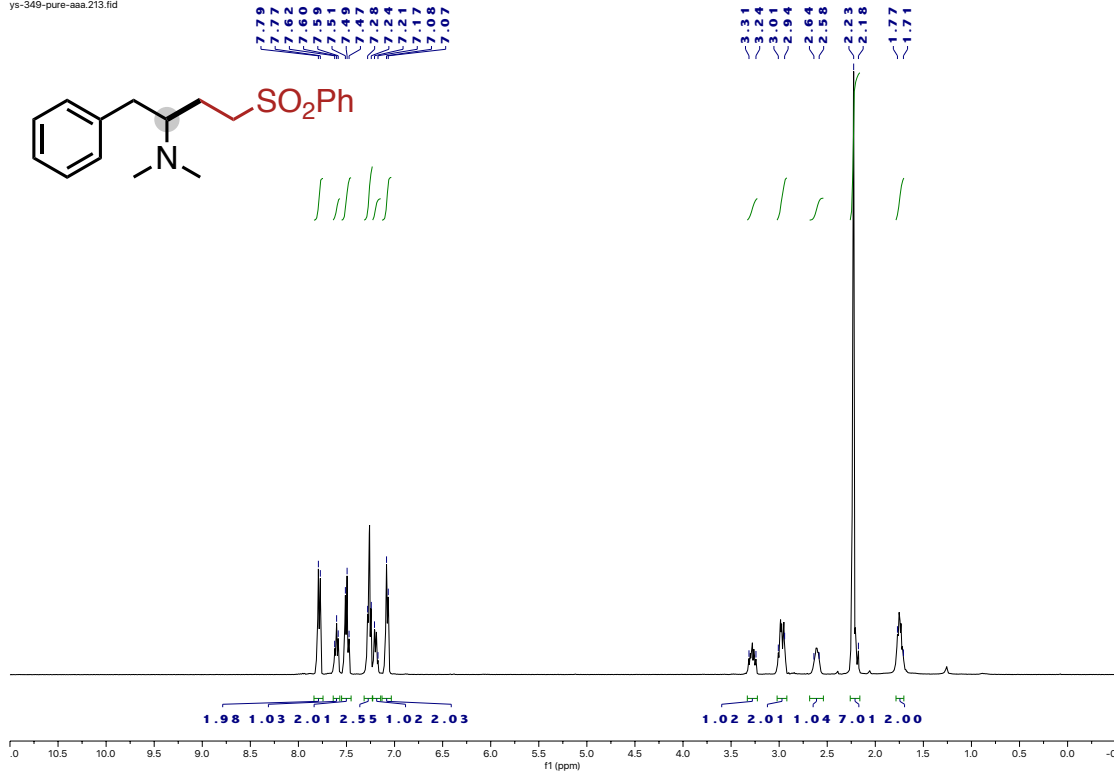
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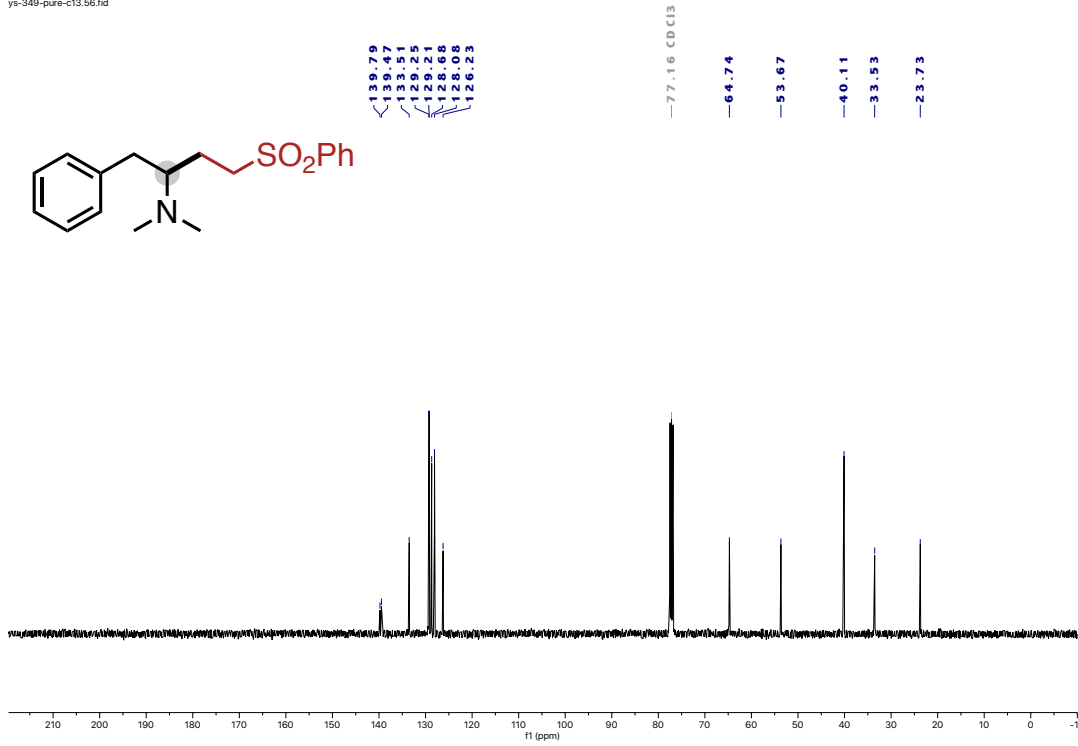
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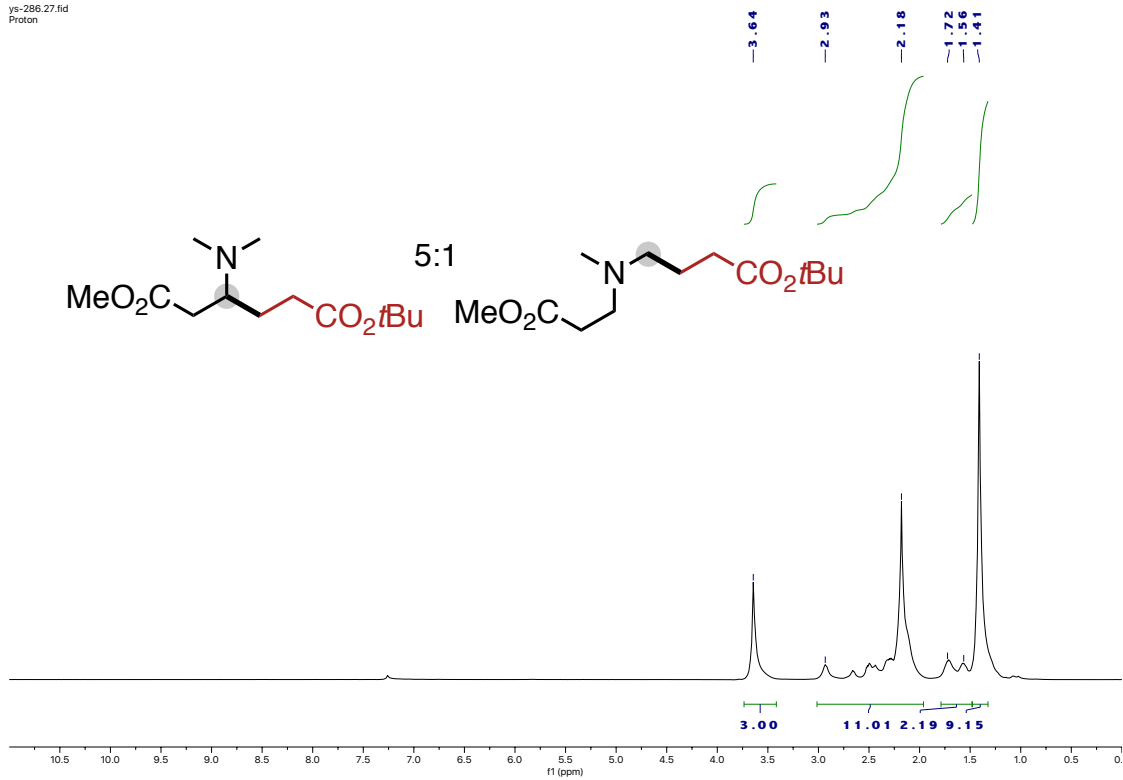
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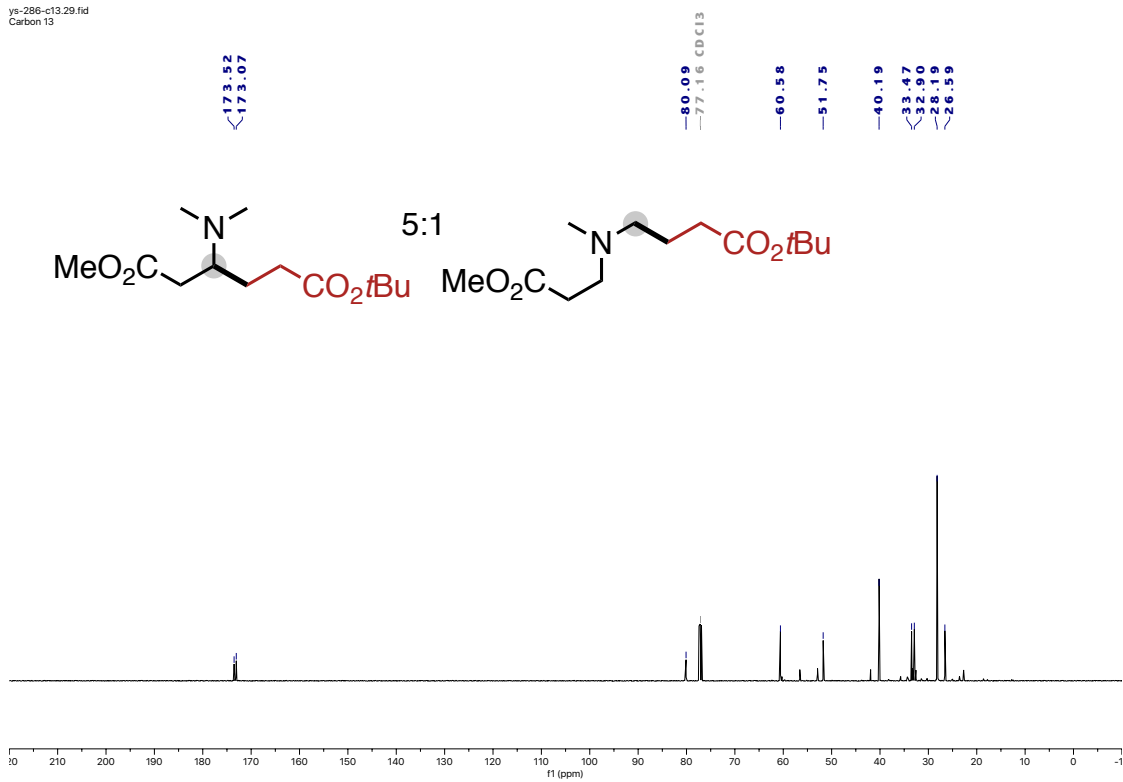
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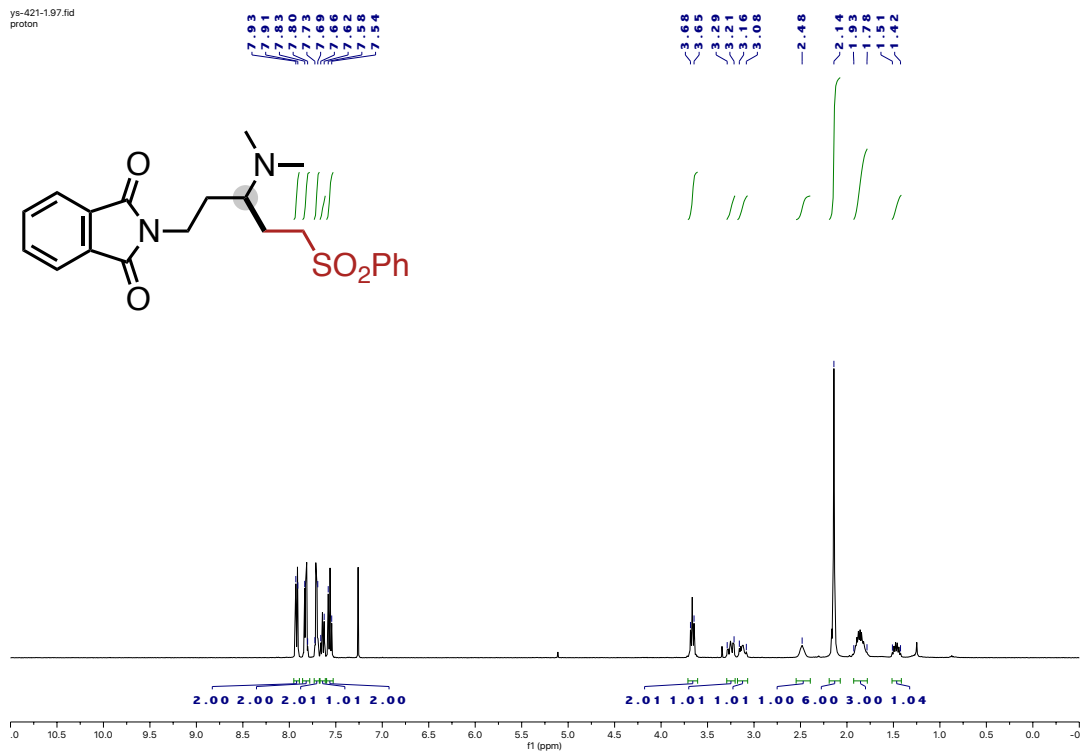
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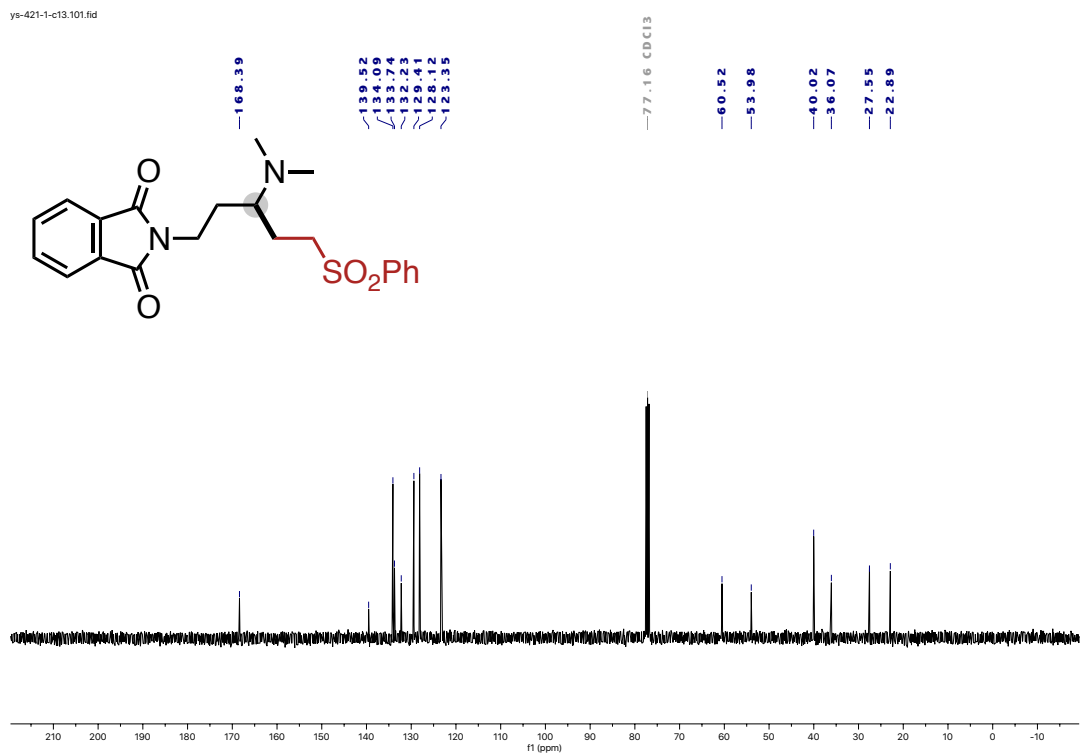
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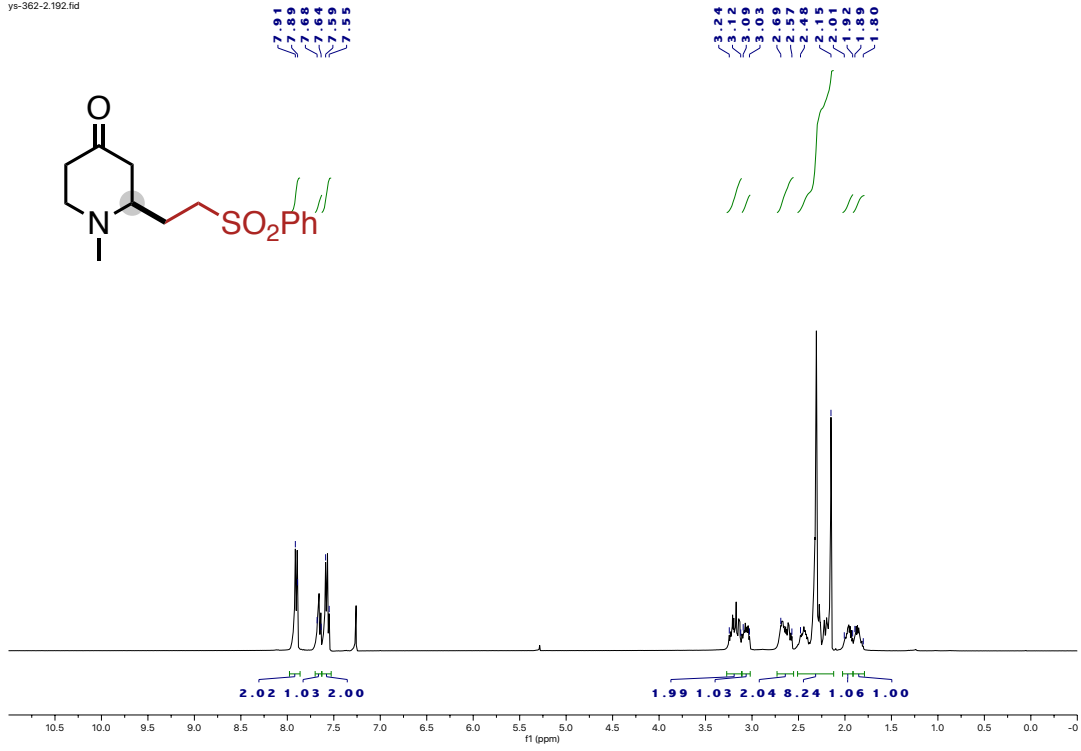
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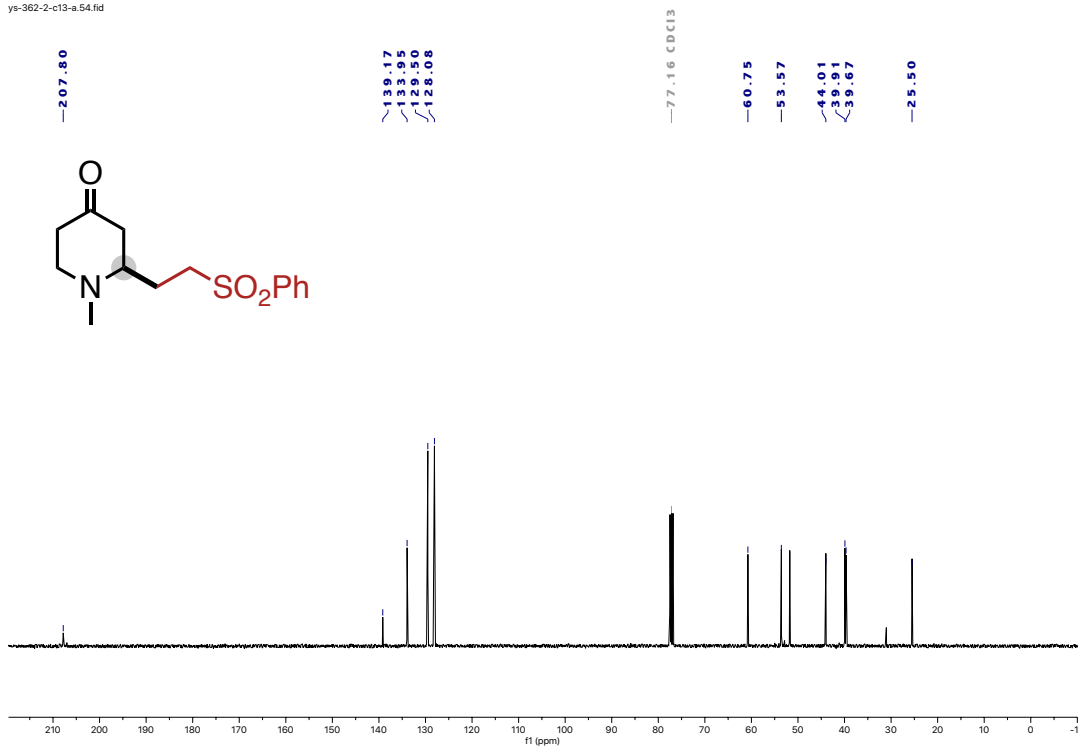
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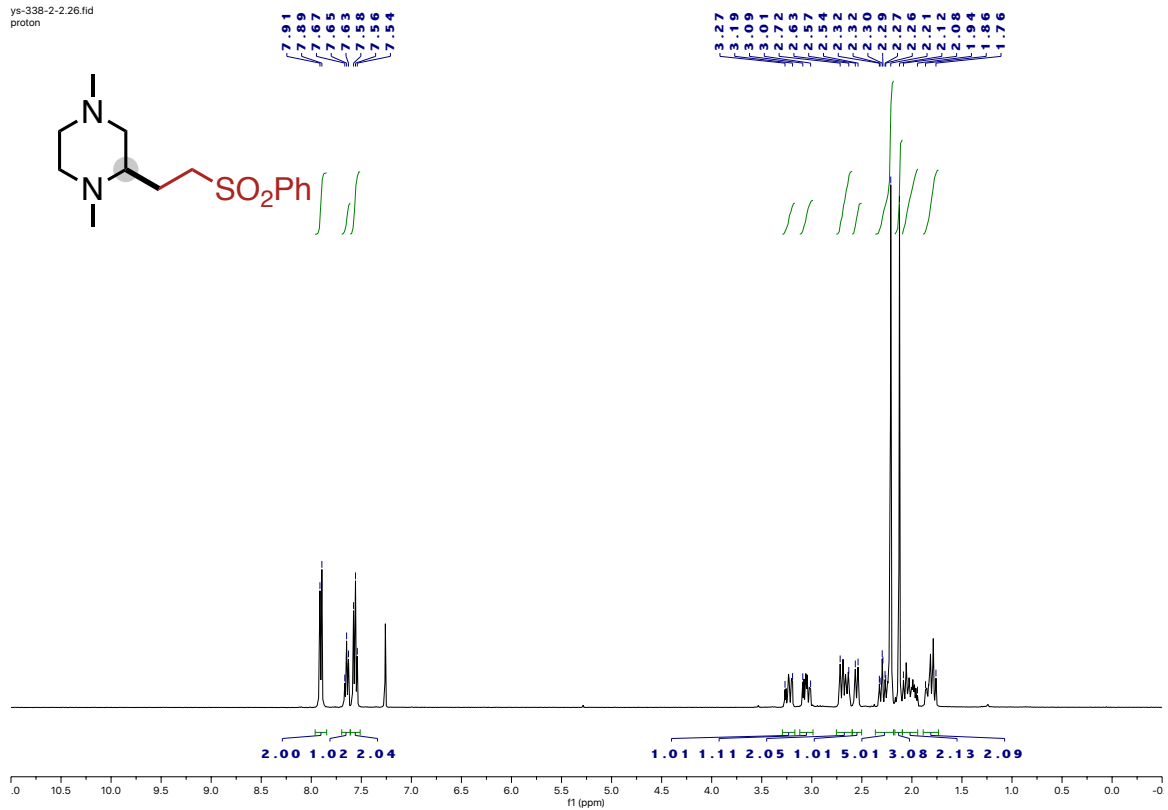
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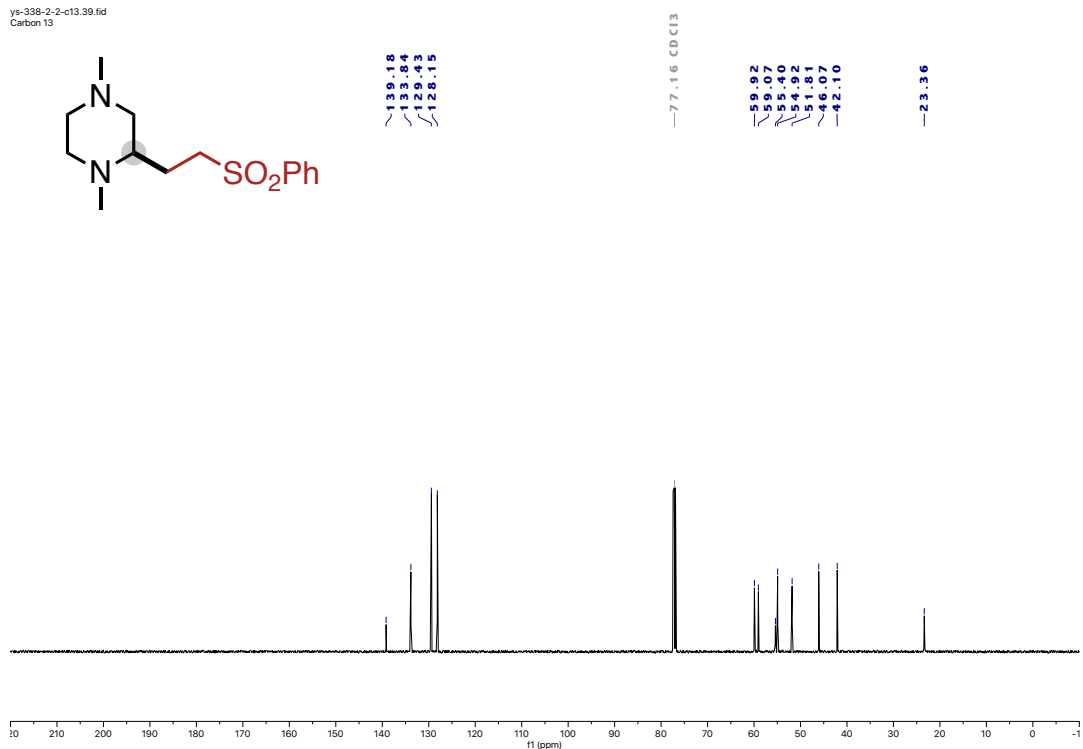
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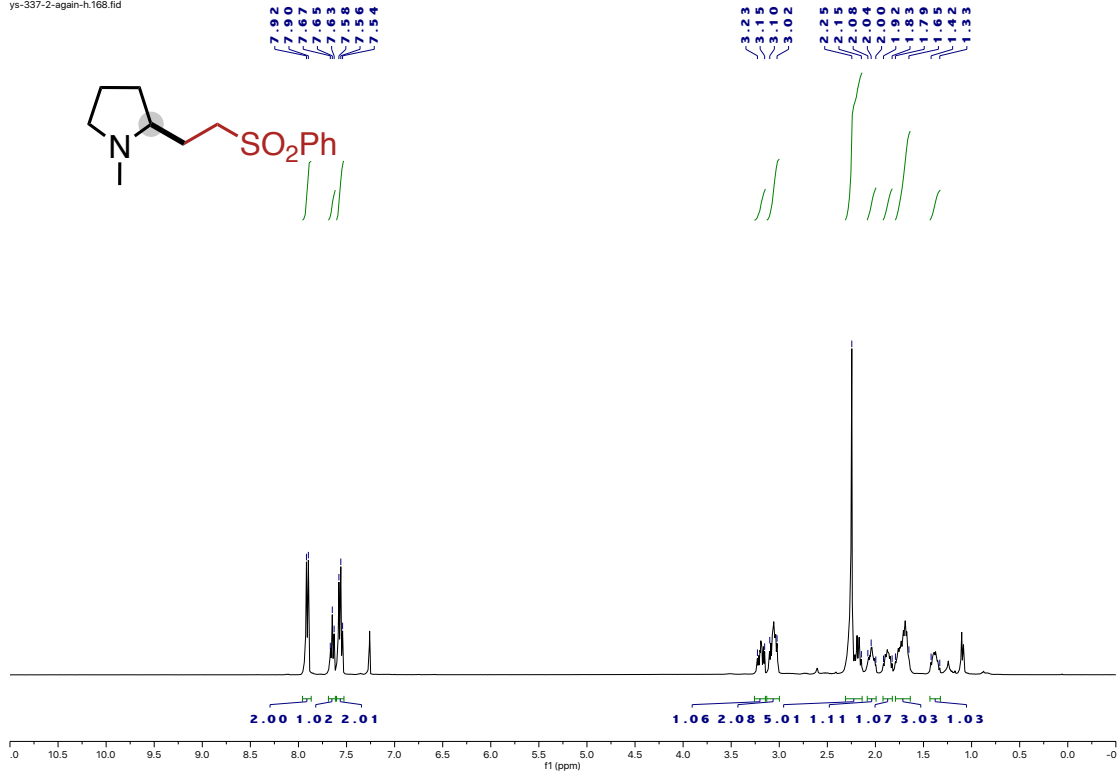
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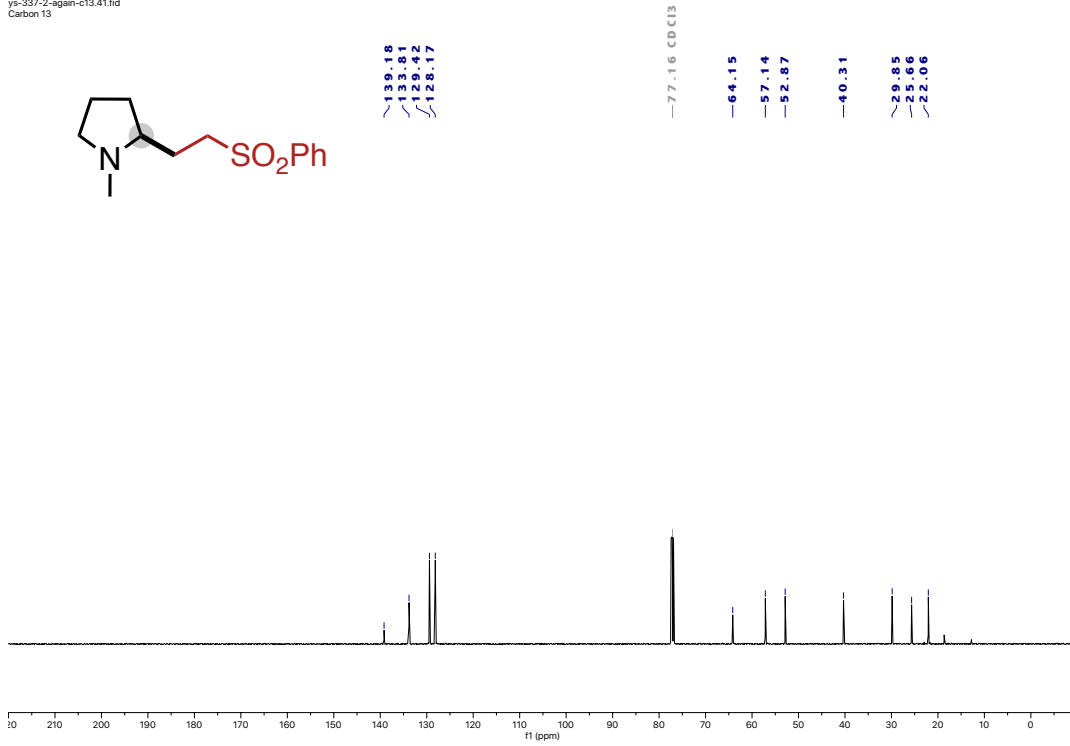
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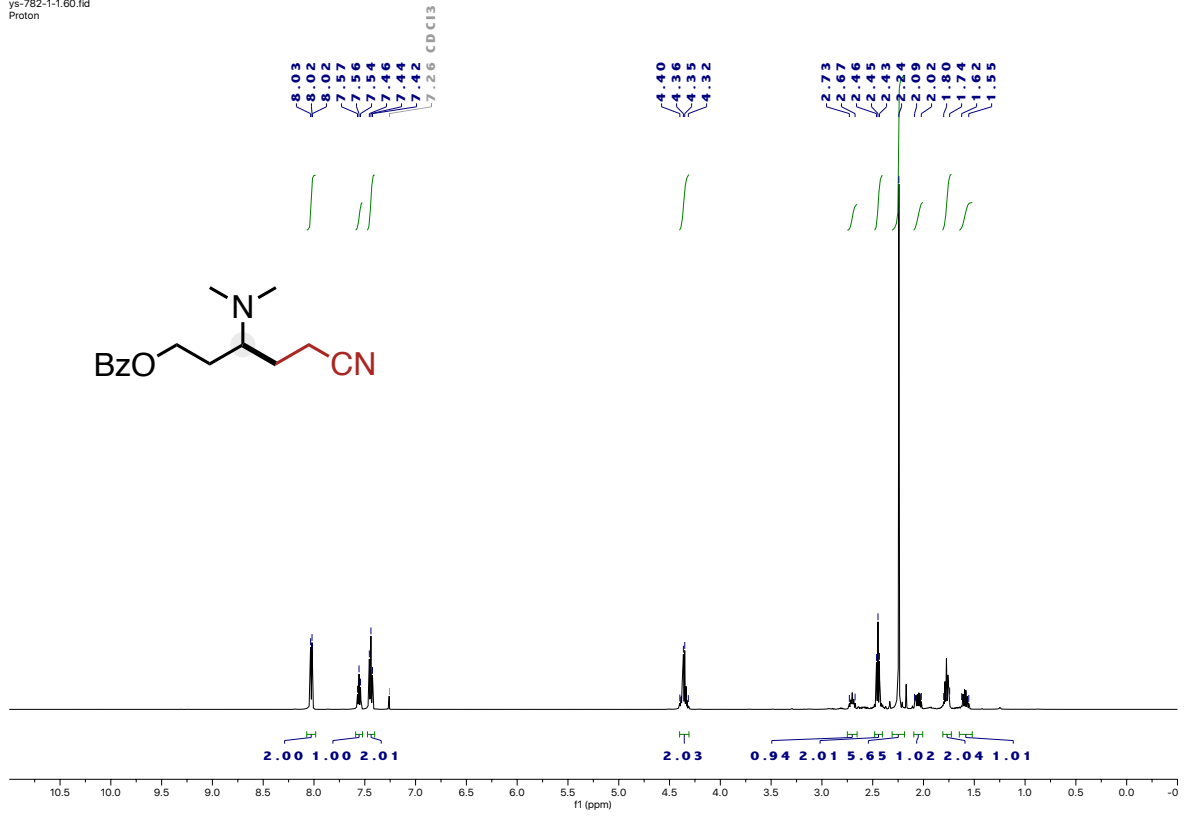
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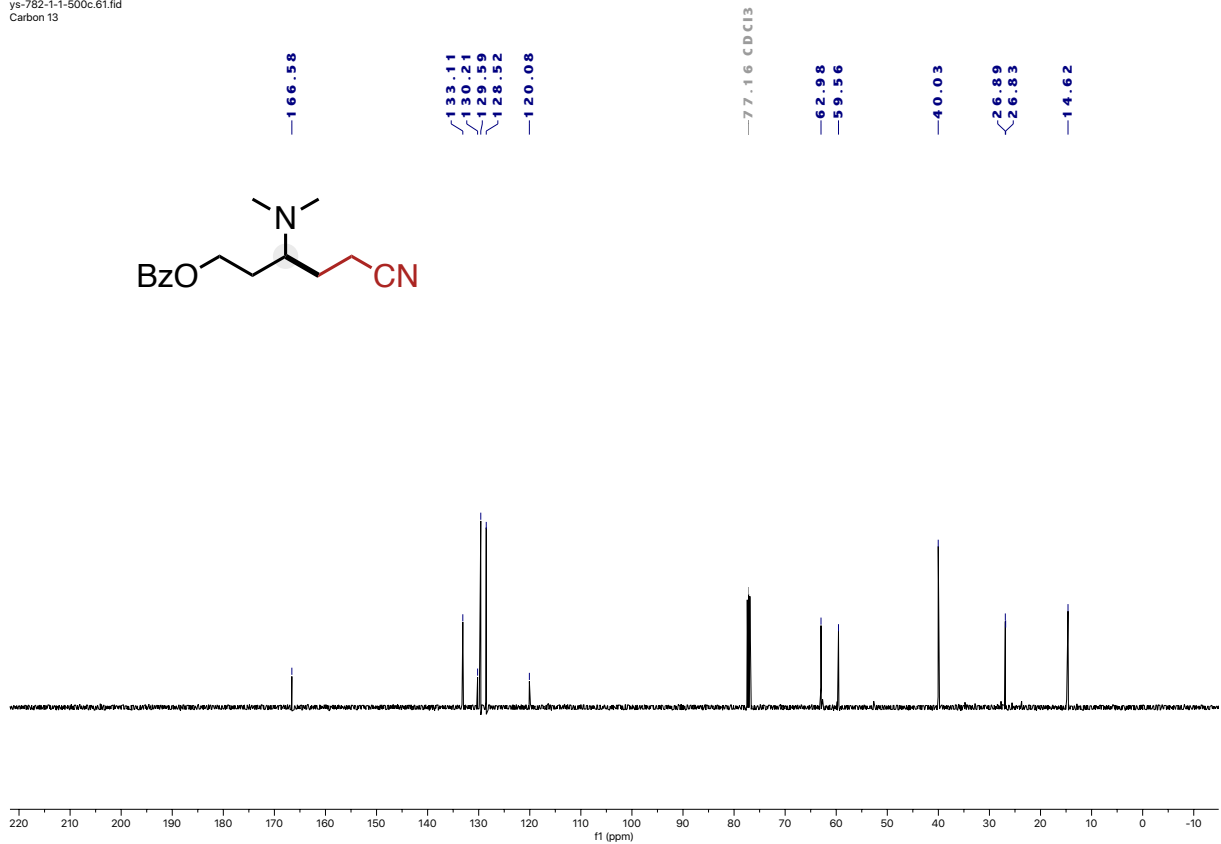
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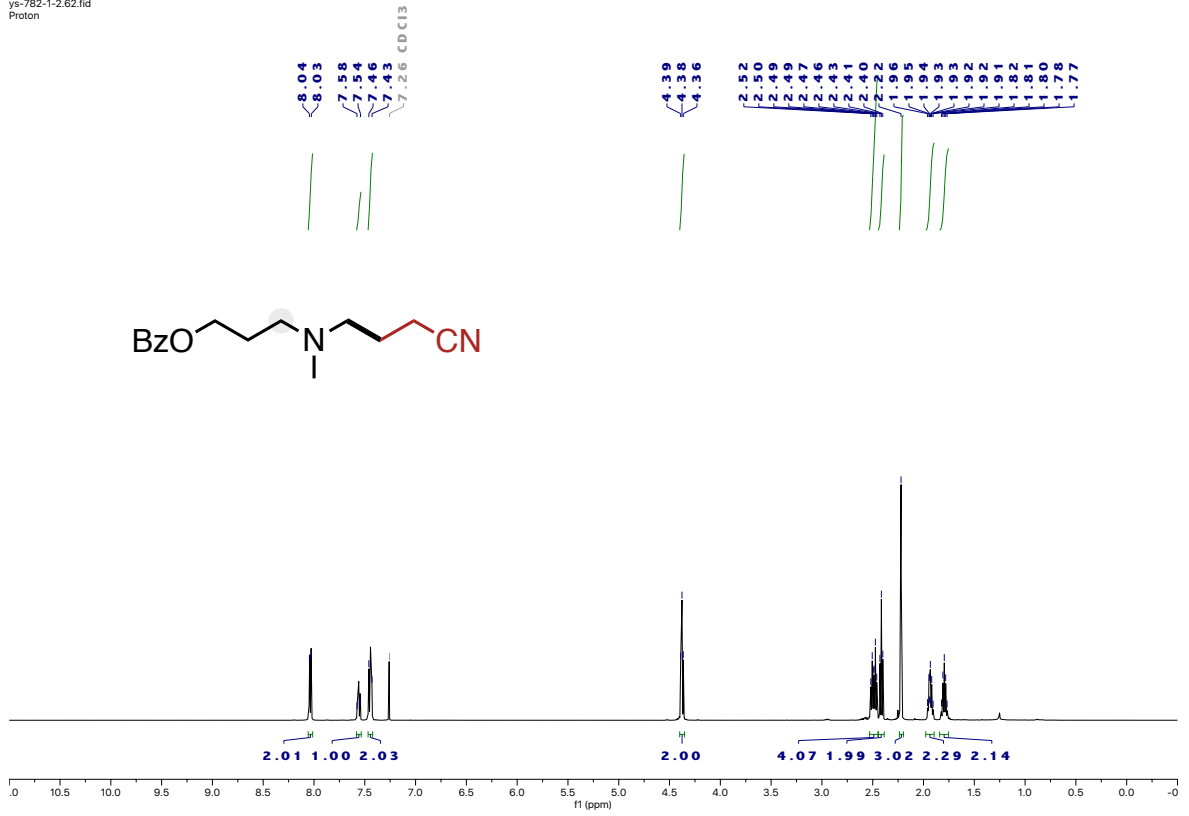
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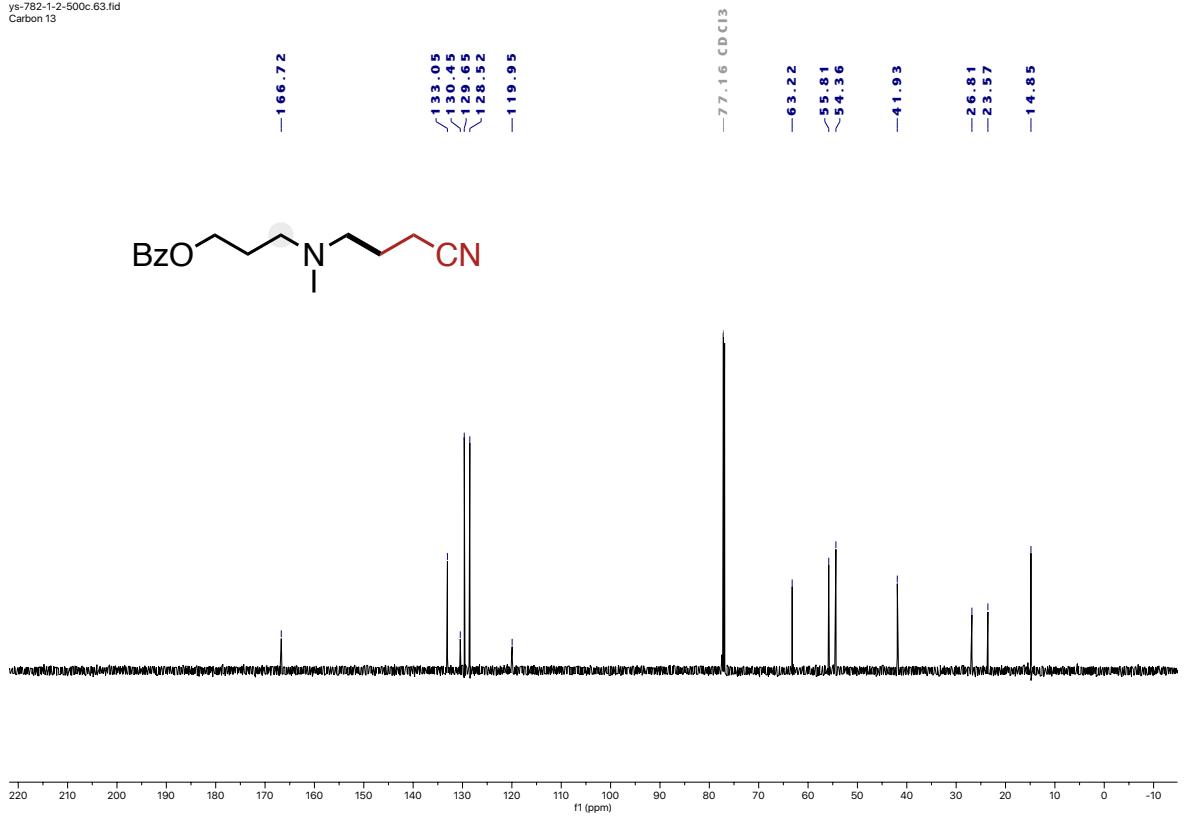
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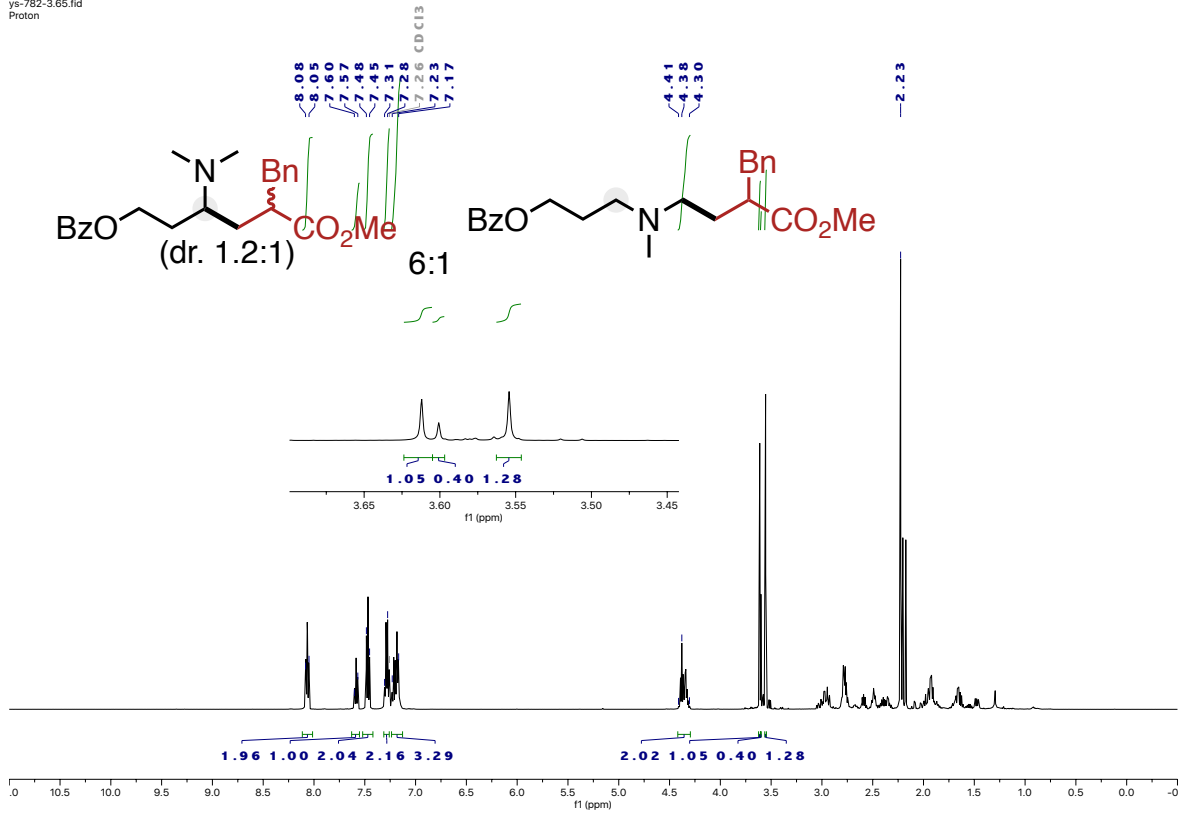
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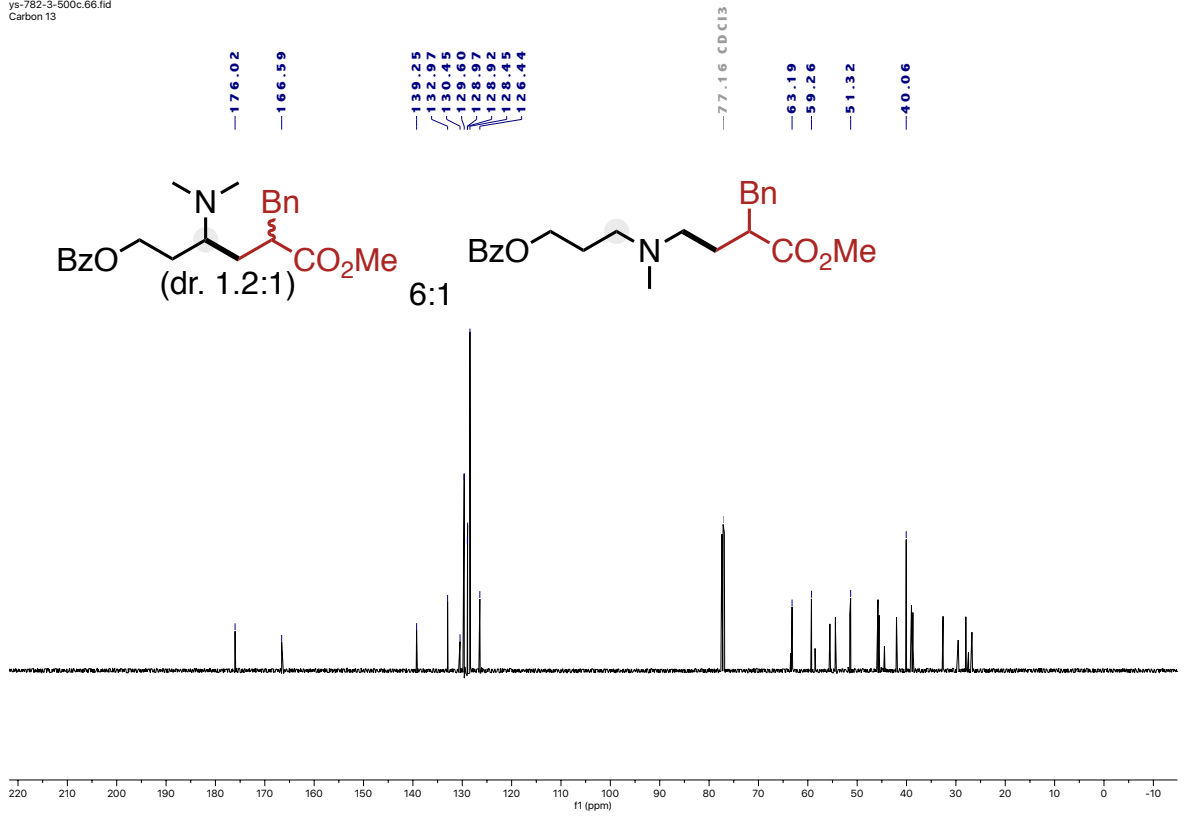
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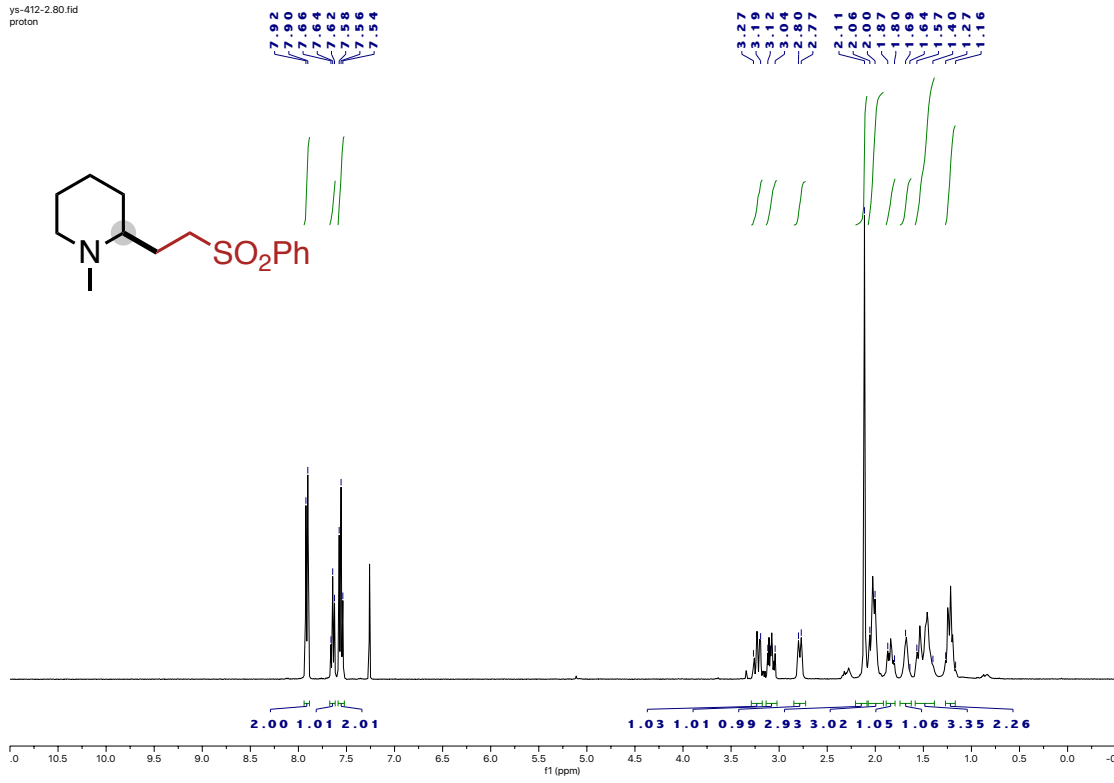
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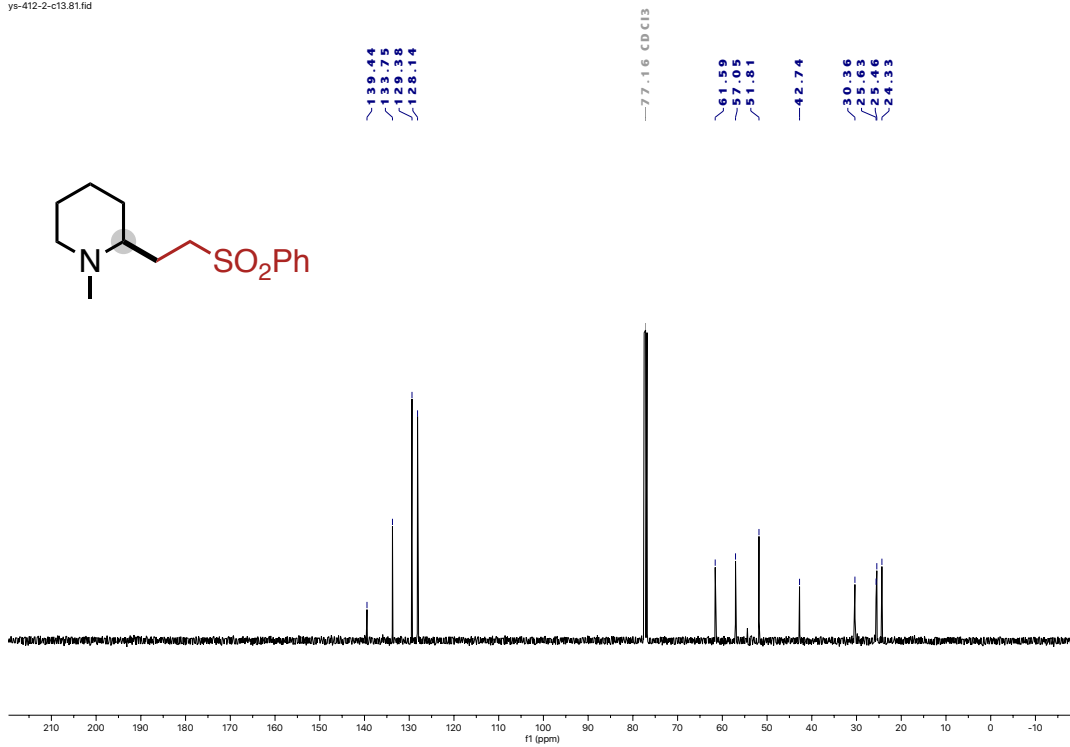
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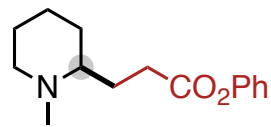
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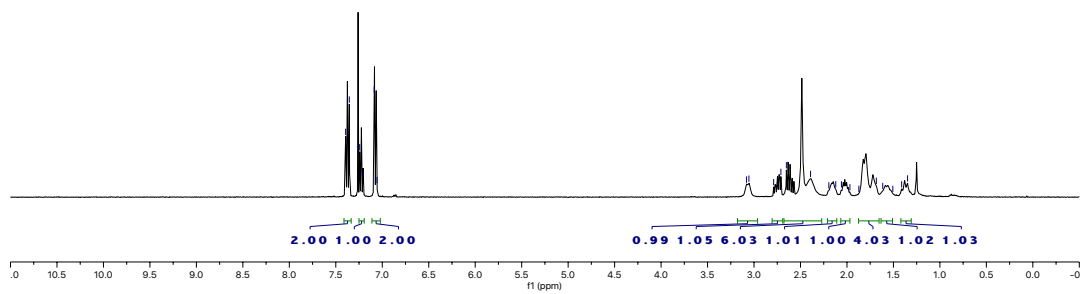


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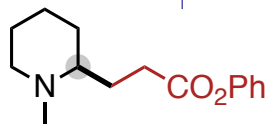


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7.09
7.06

3.08
3.06
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2.71
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2.39
2.19
2.06
1.97
1.87
1.68
1.51
1.31



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129.58

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63.16

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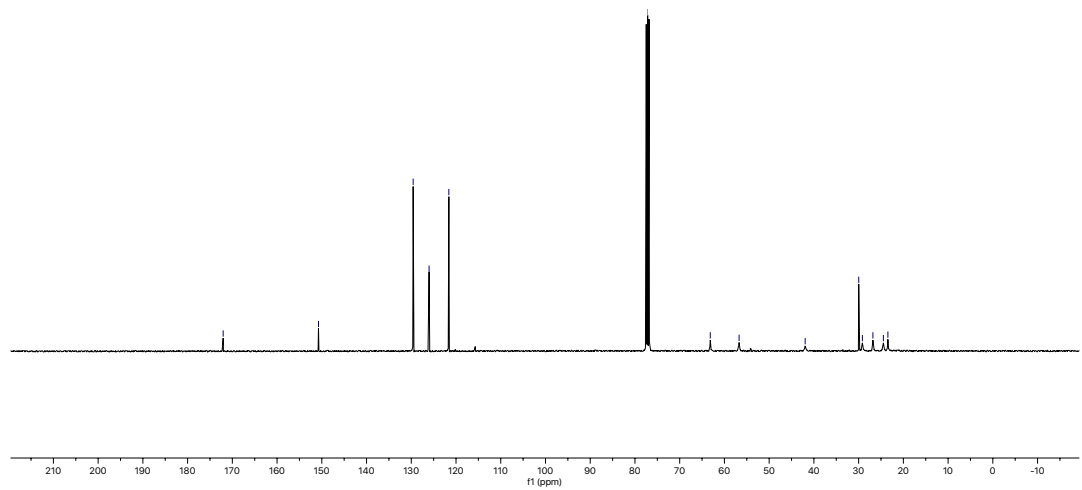
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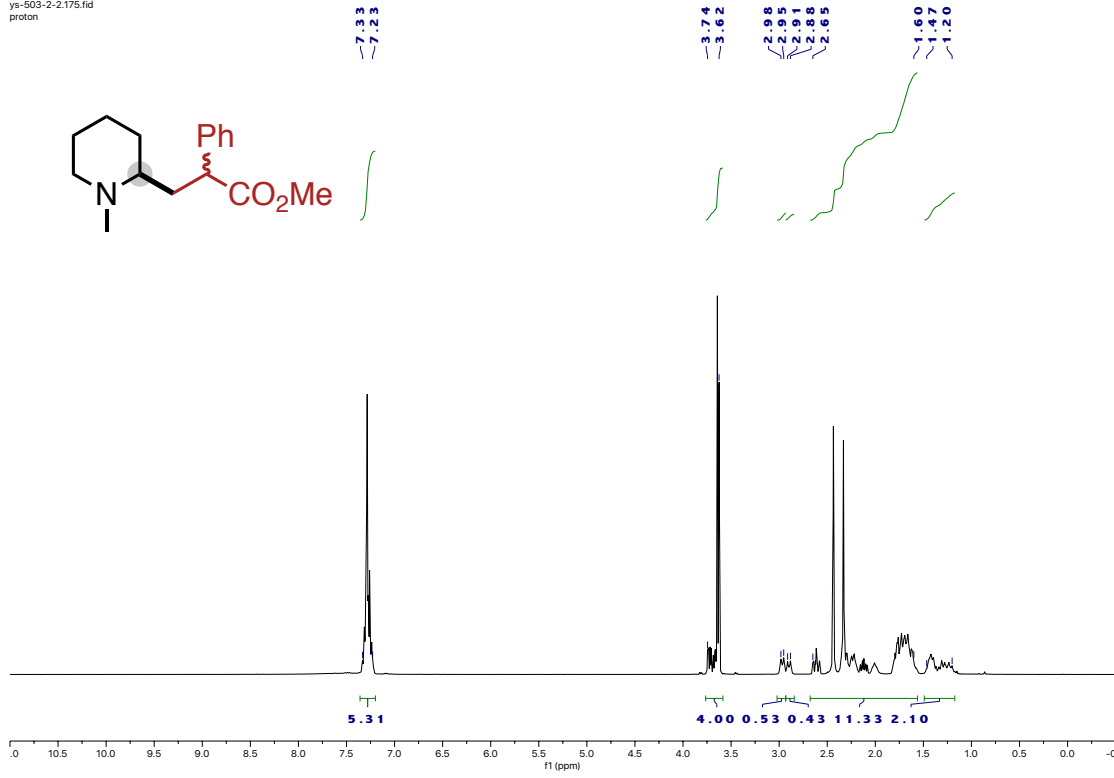
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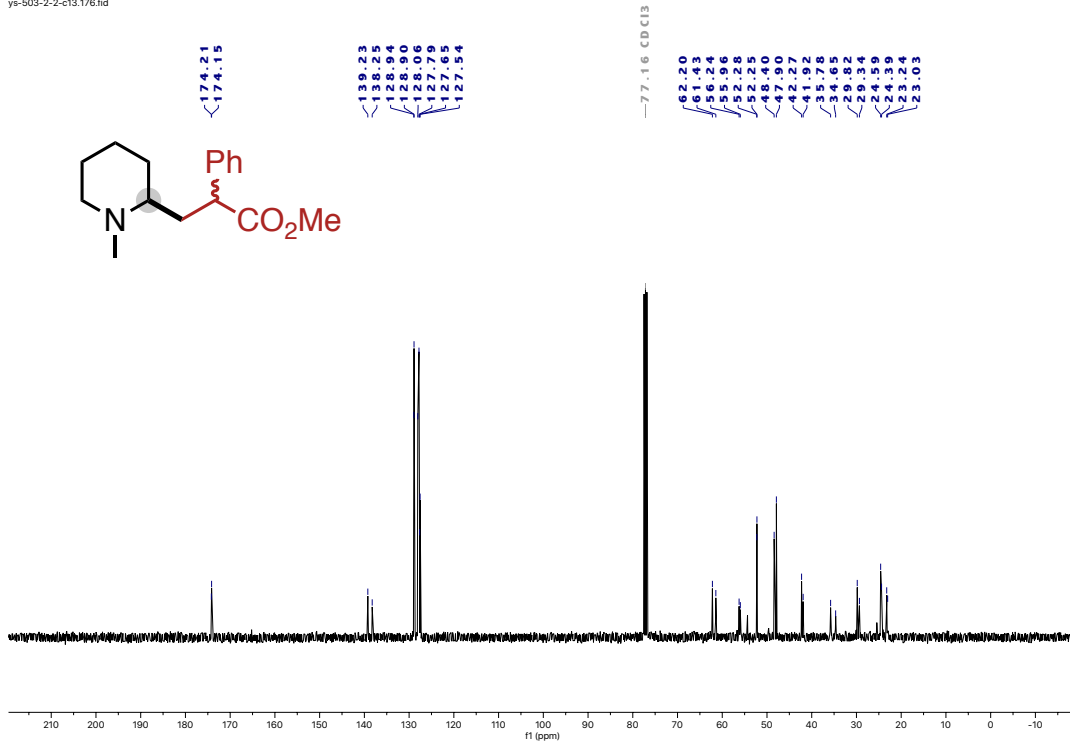
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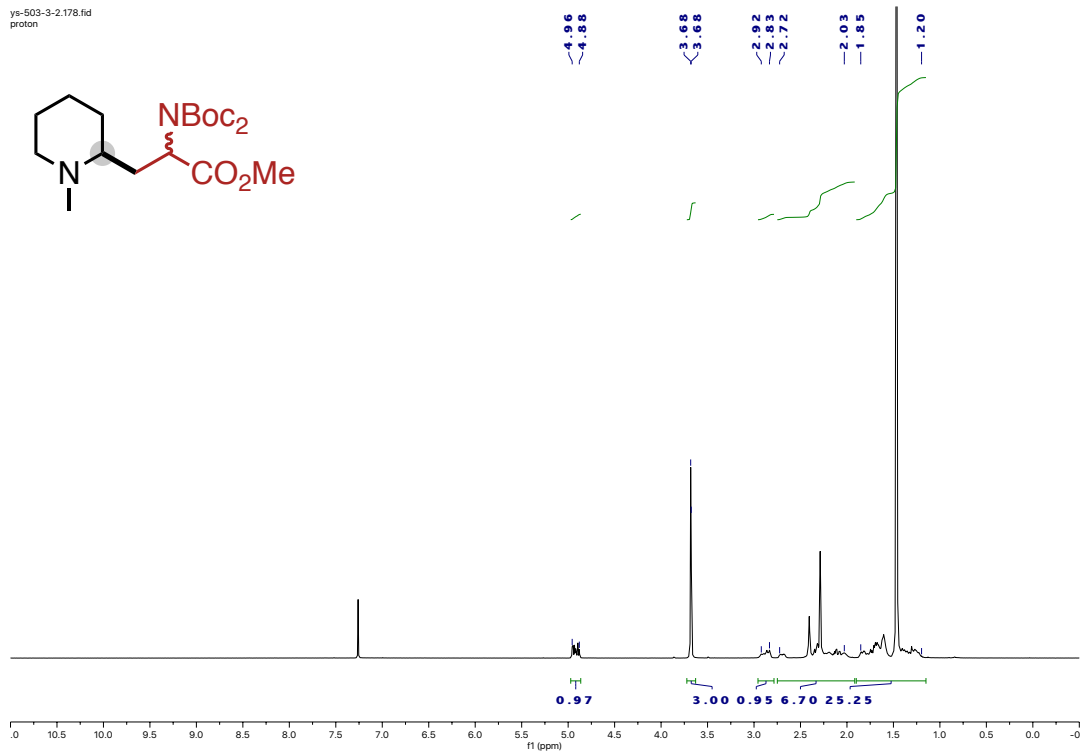
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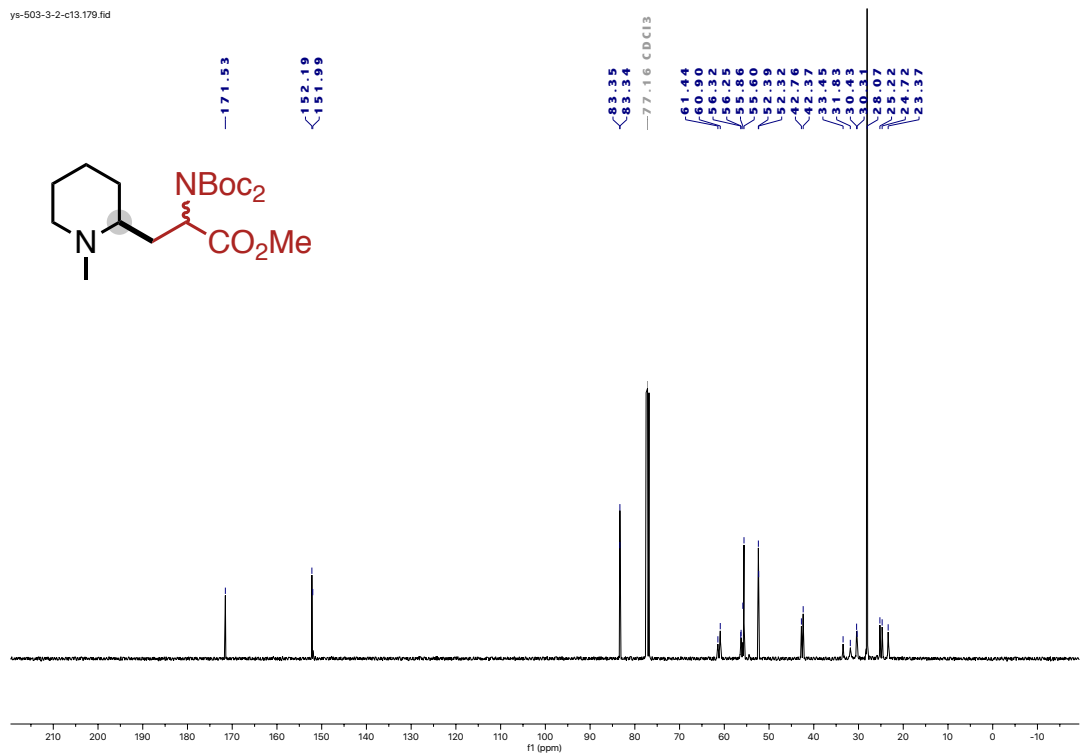
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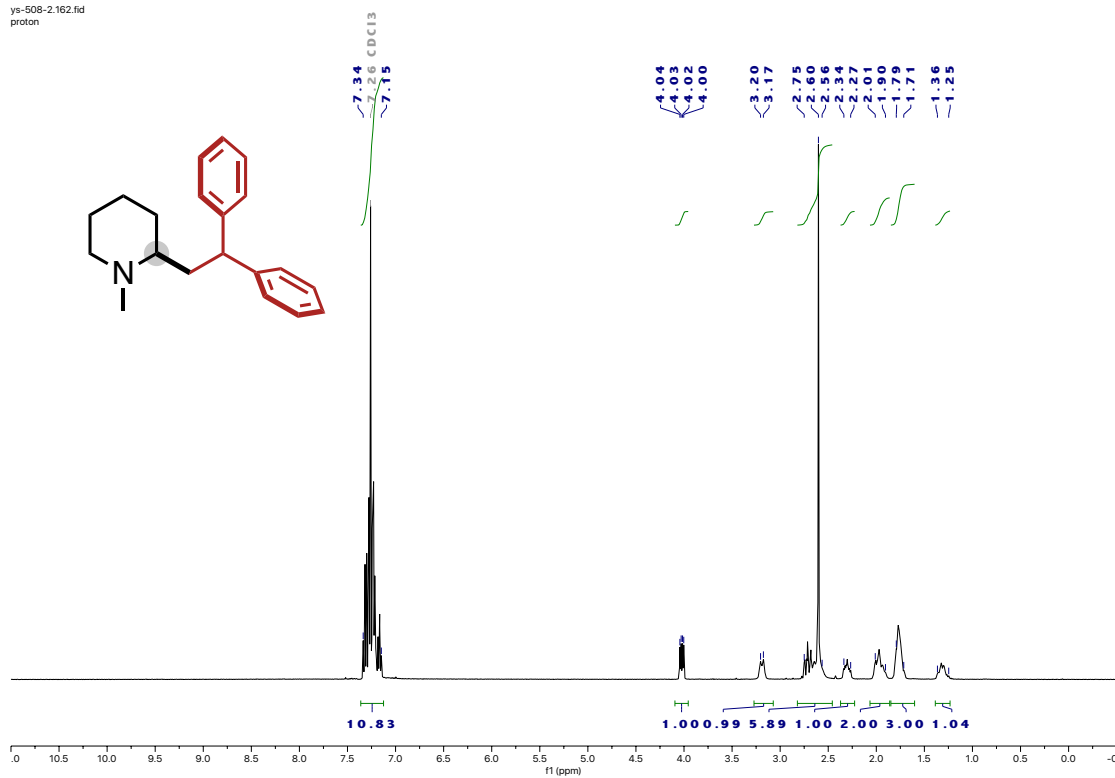
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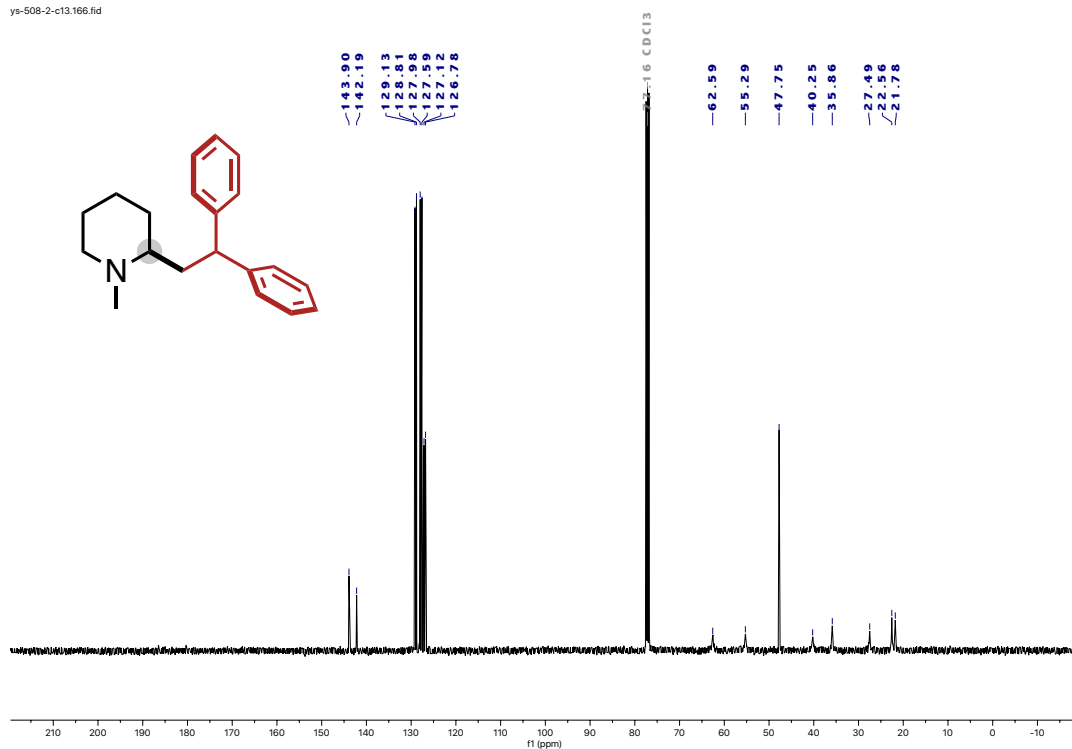
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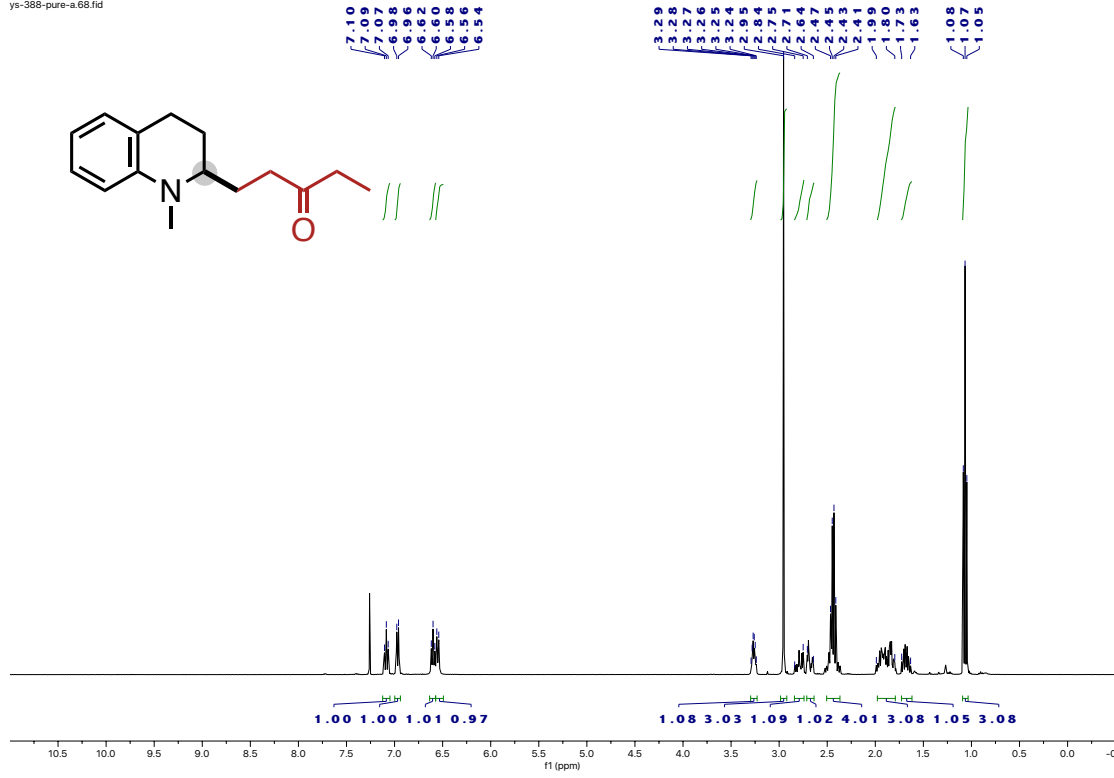
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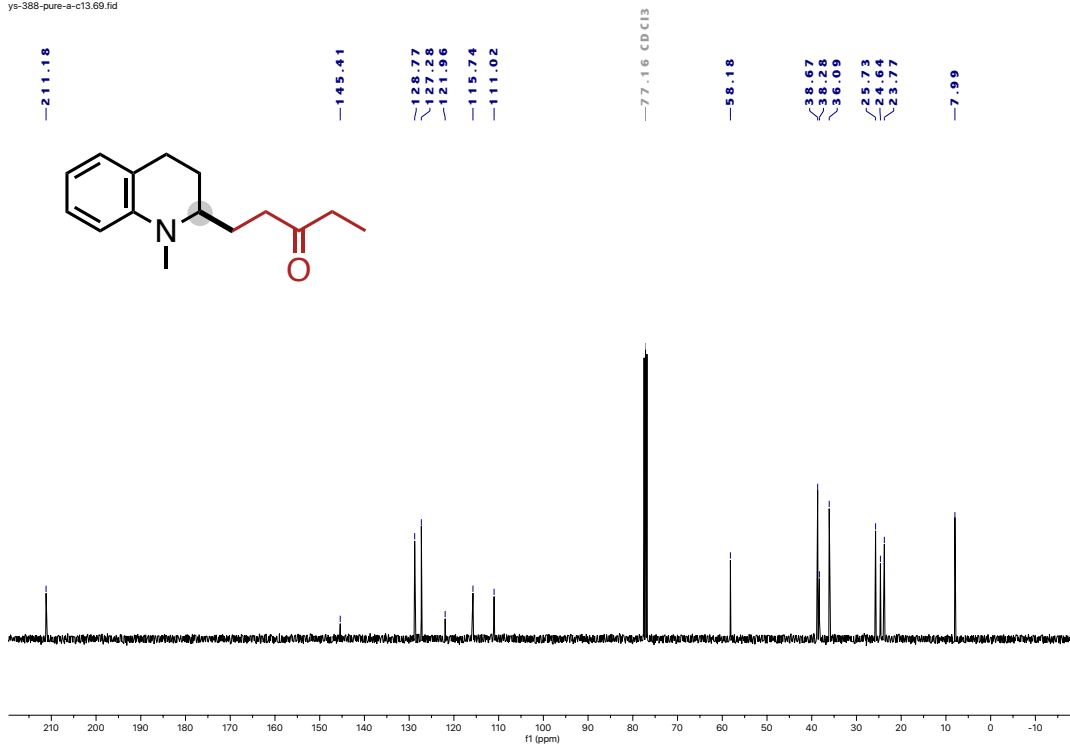
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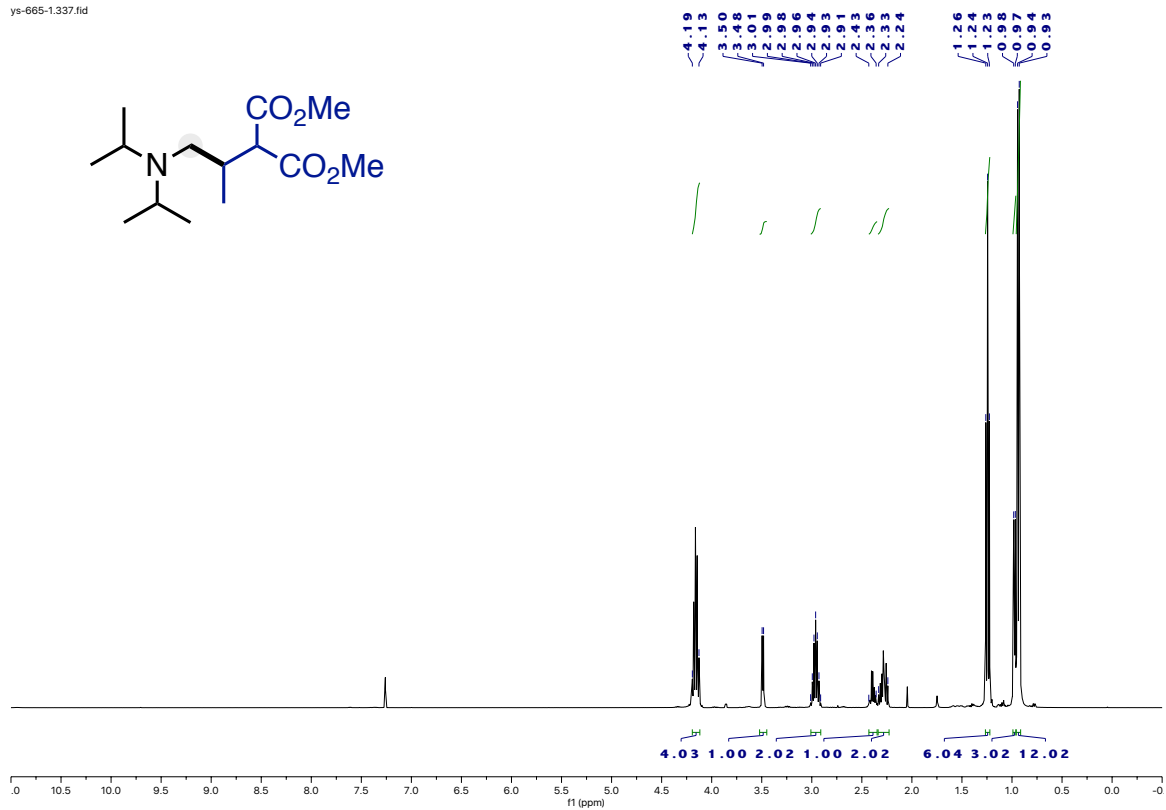
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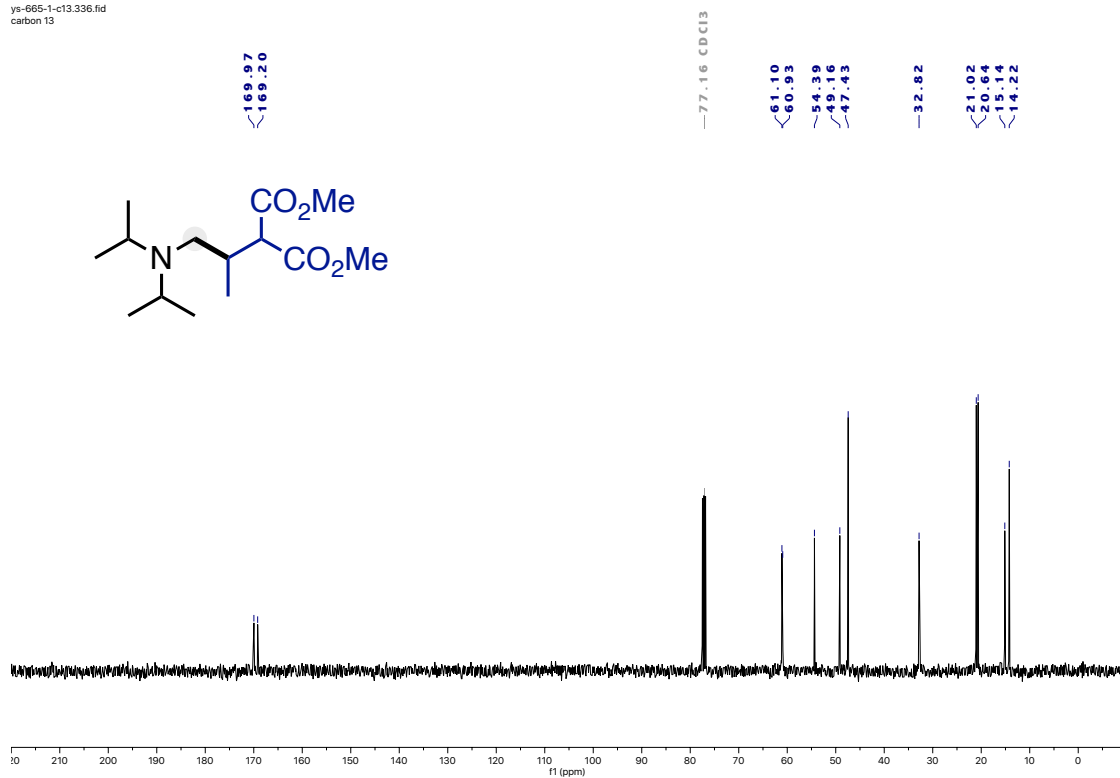
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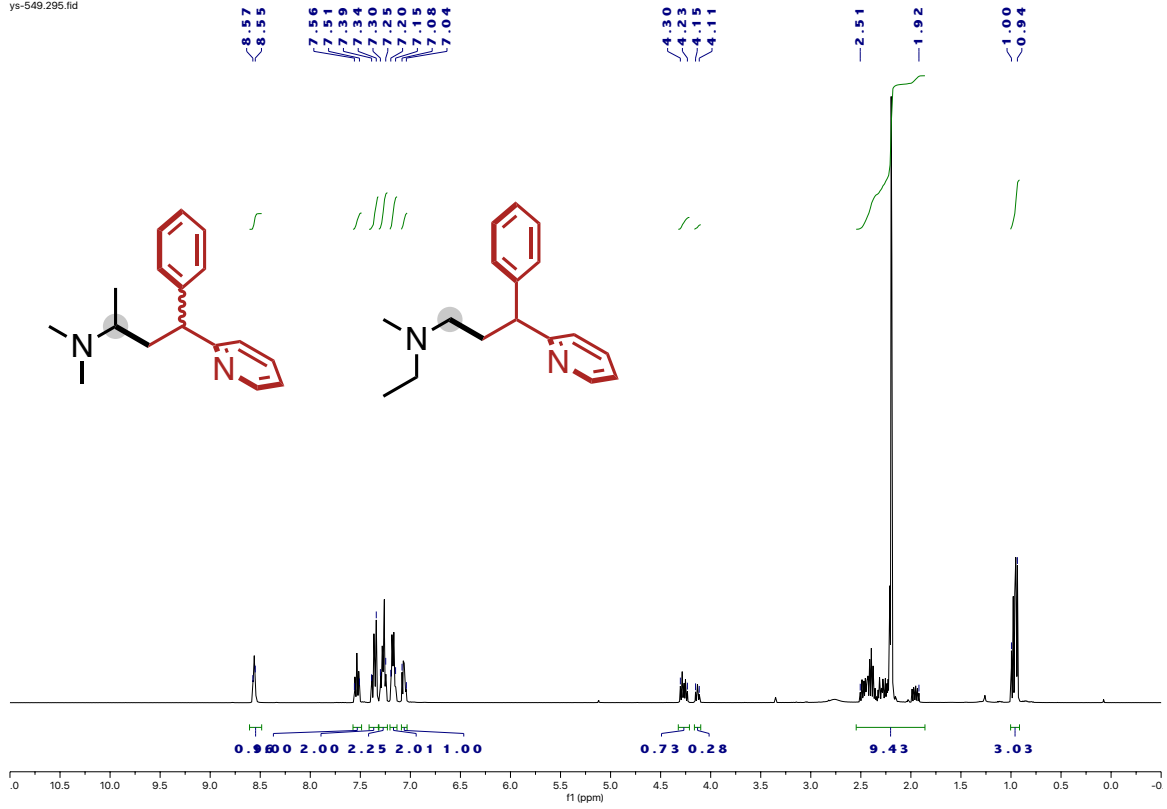
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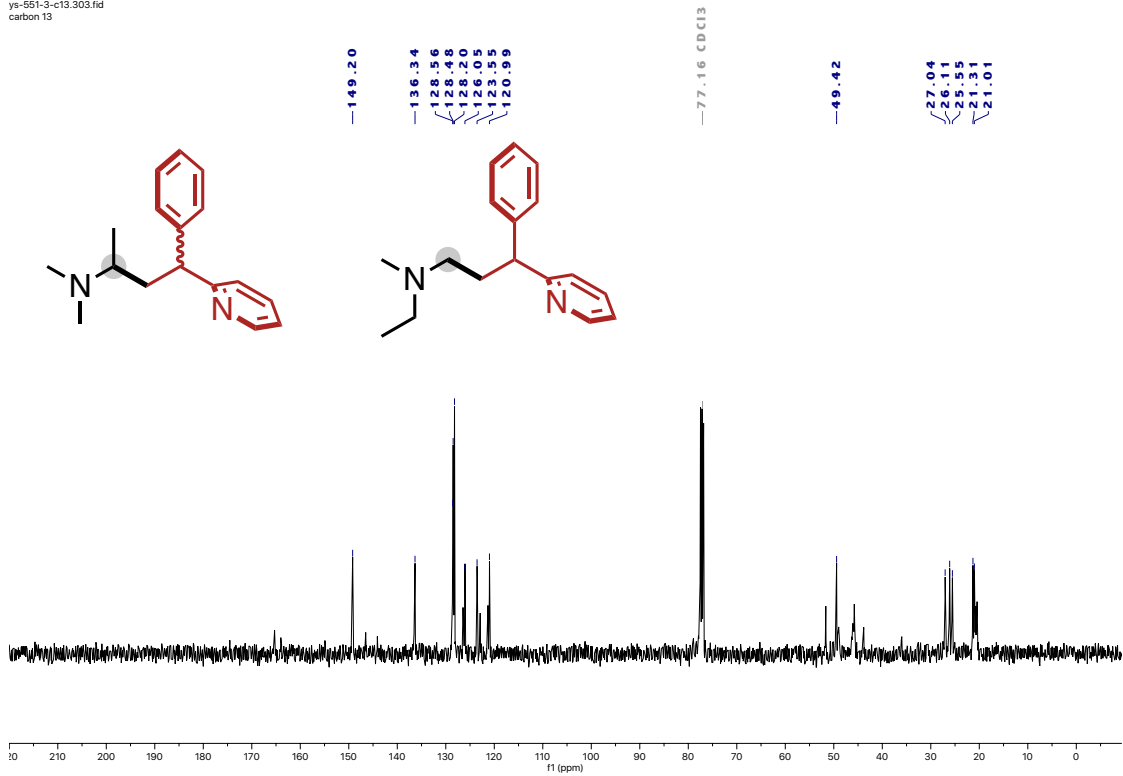
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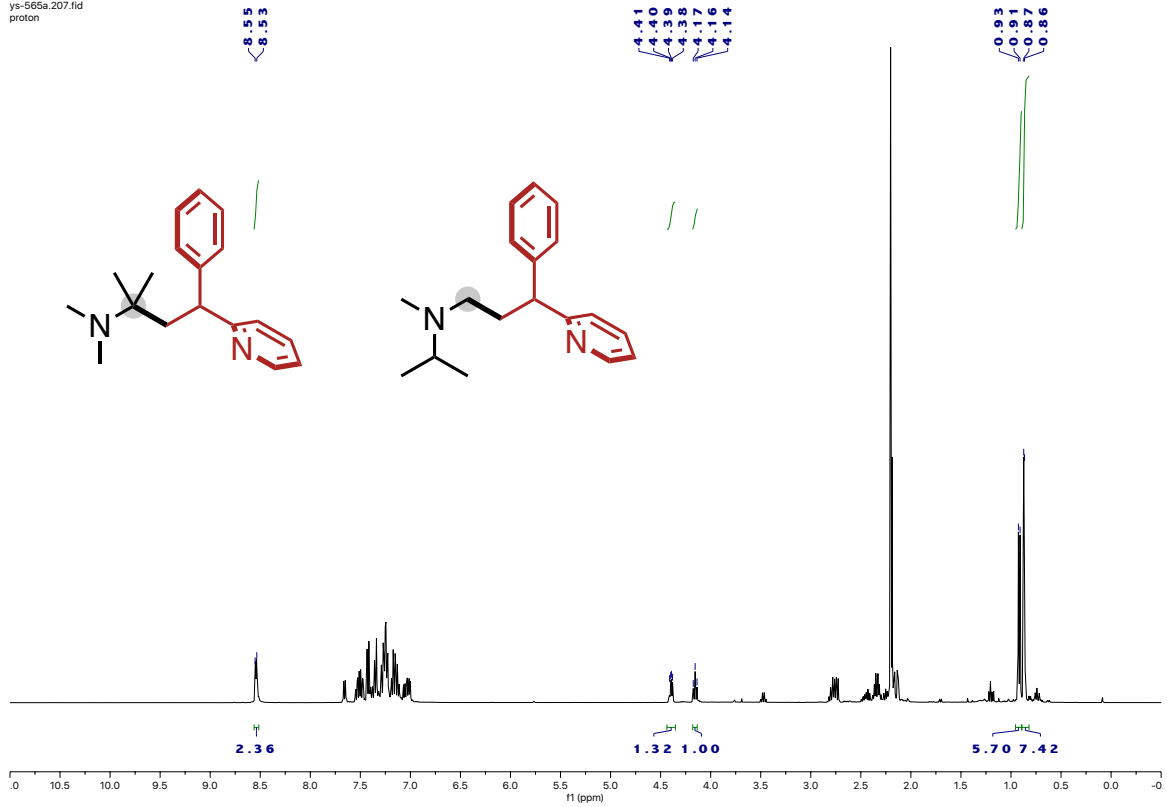
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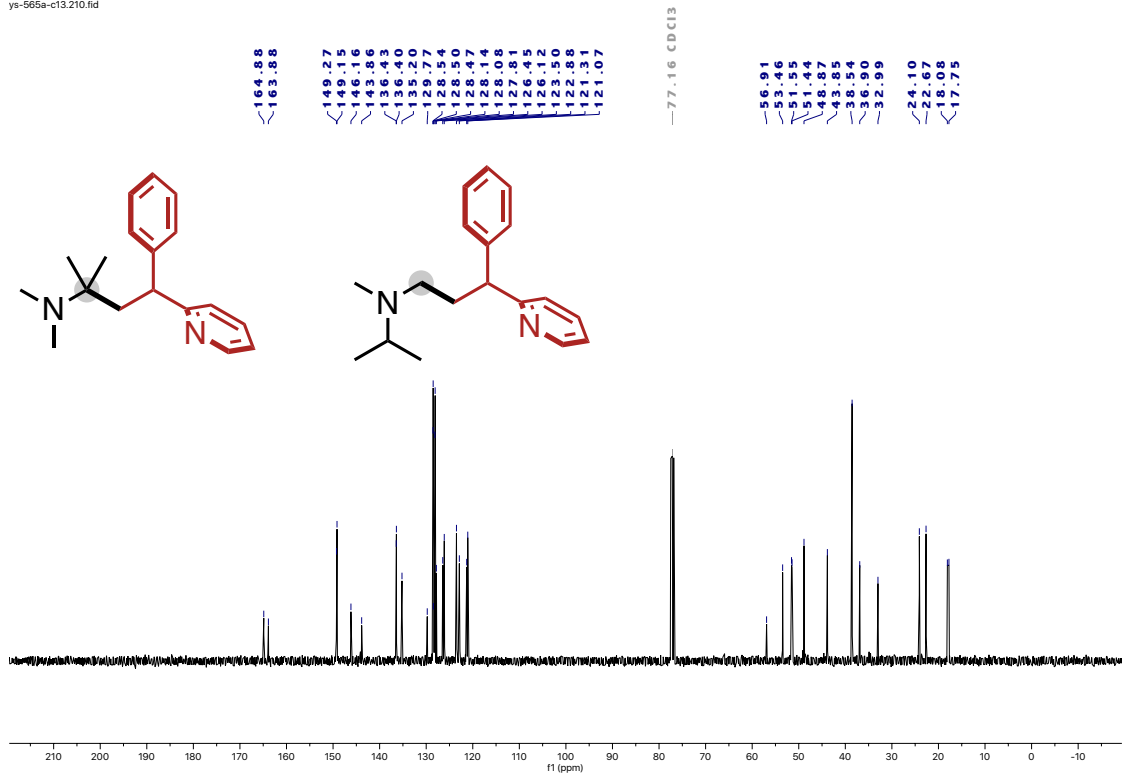
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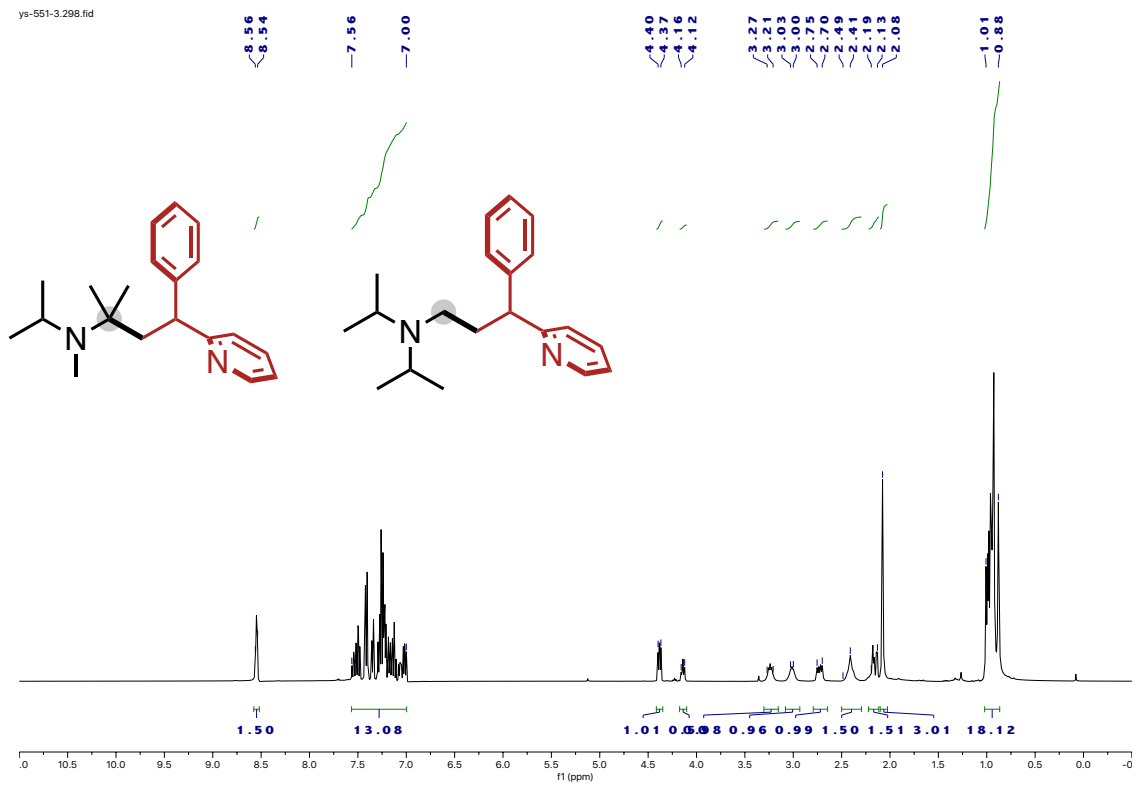
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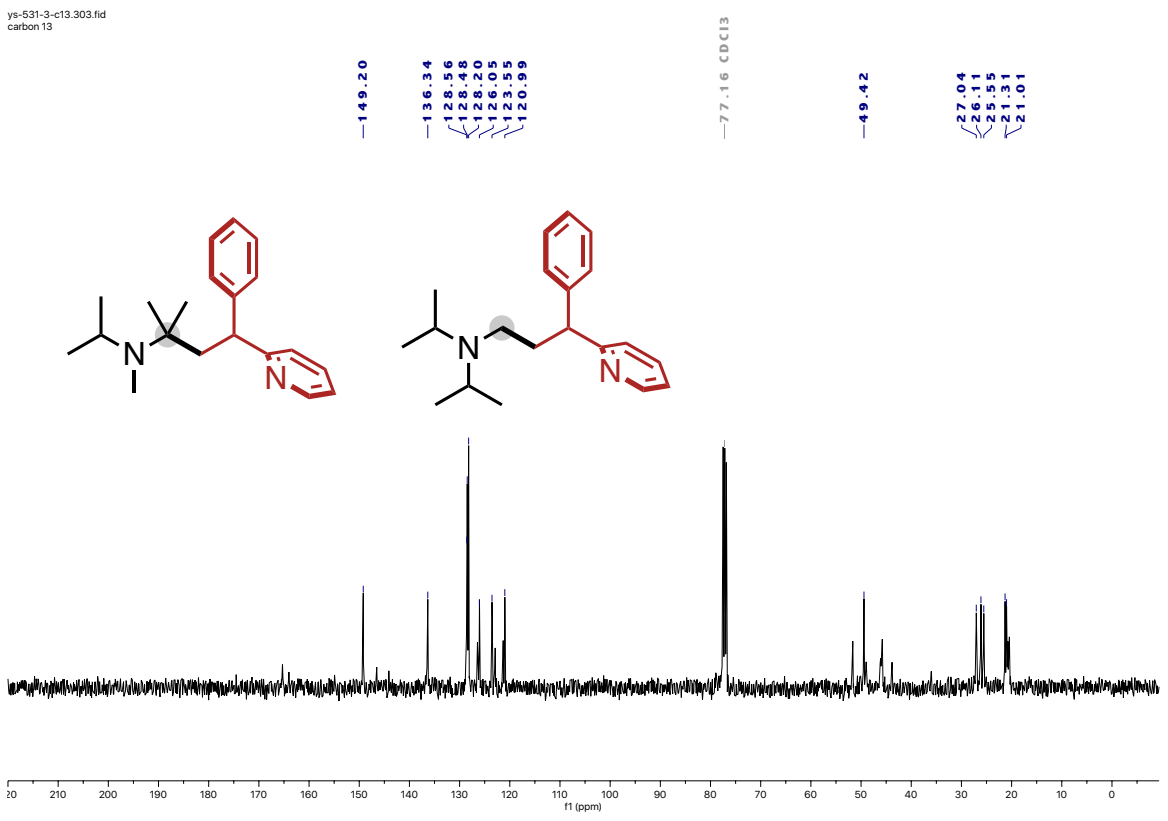
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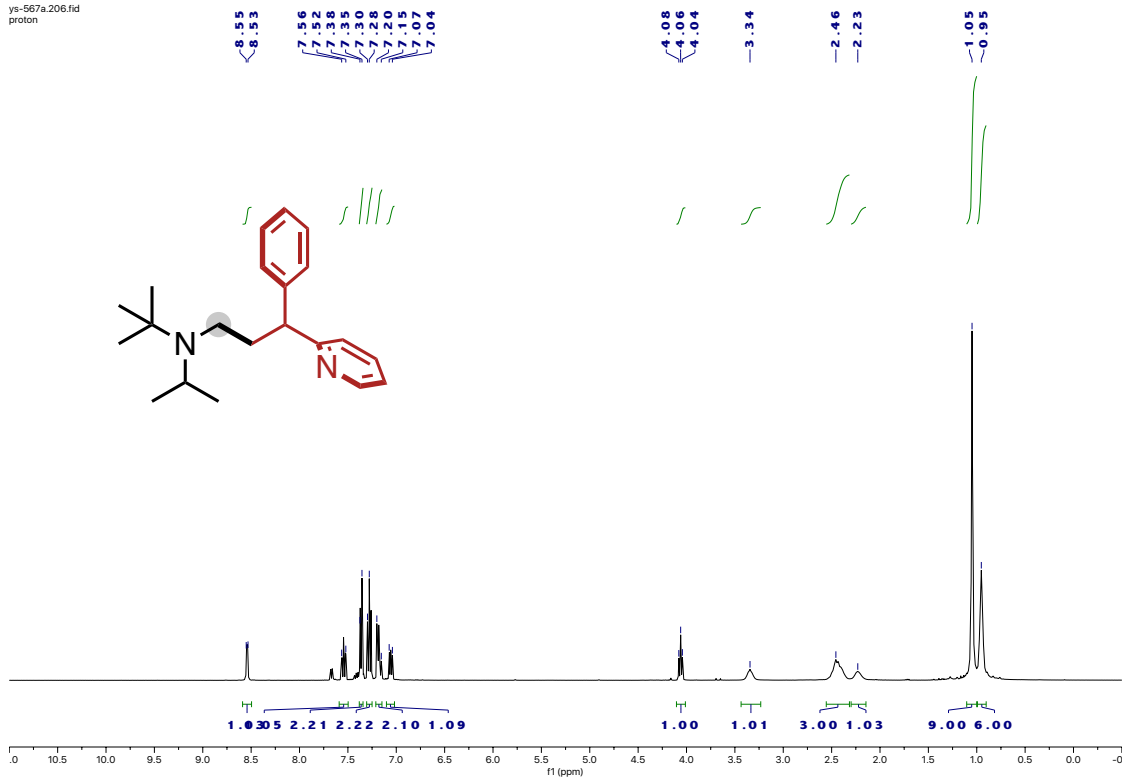
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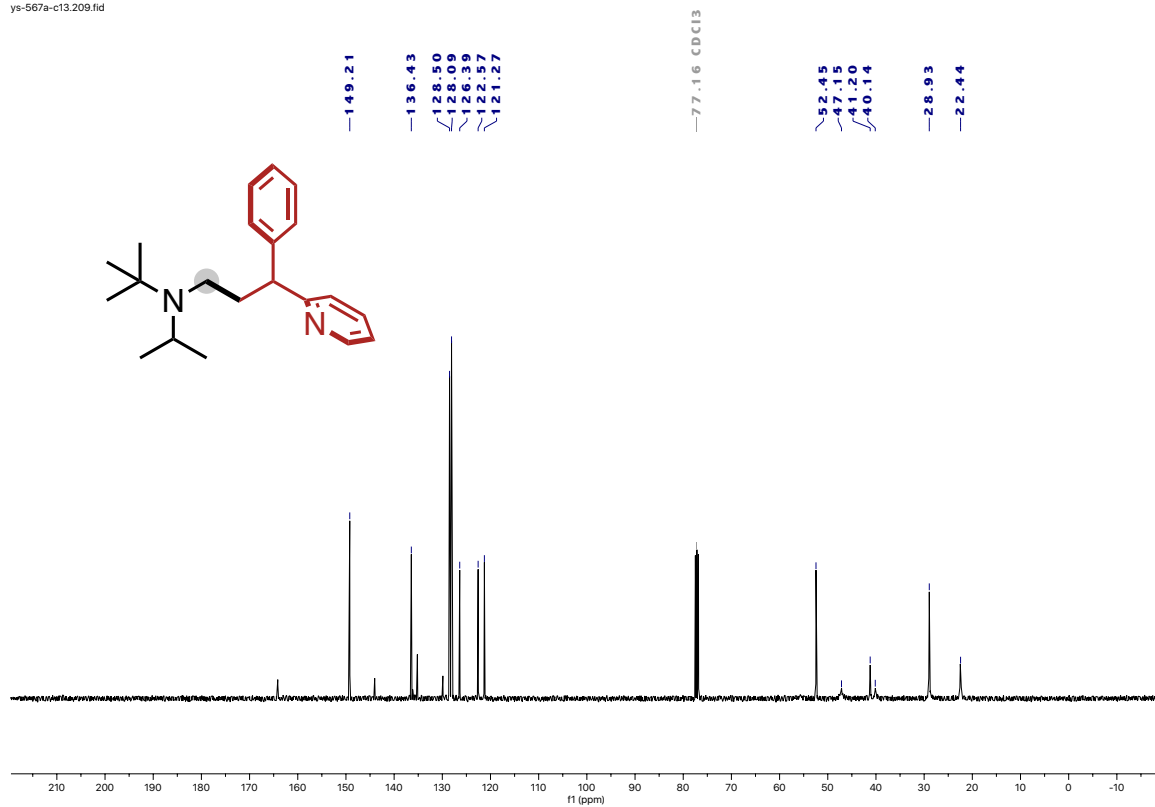
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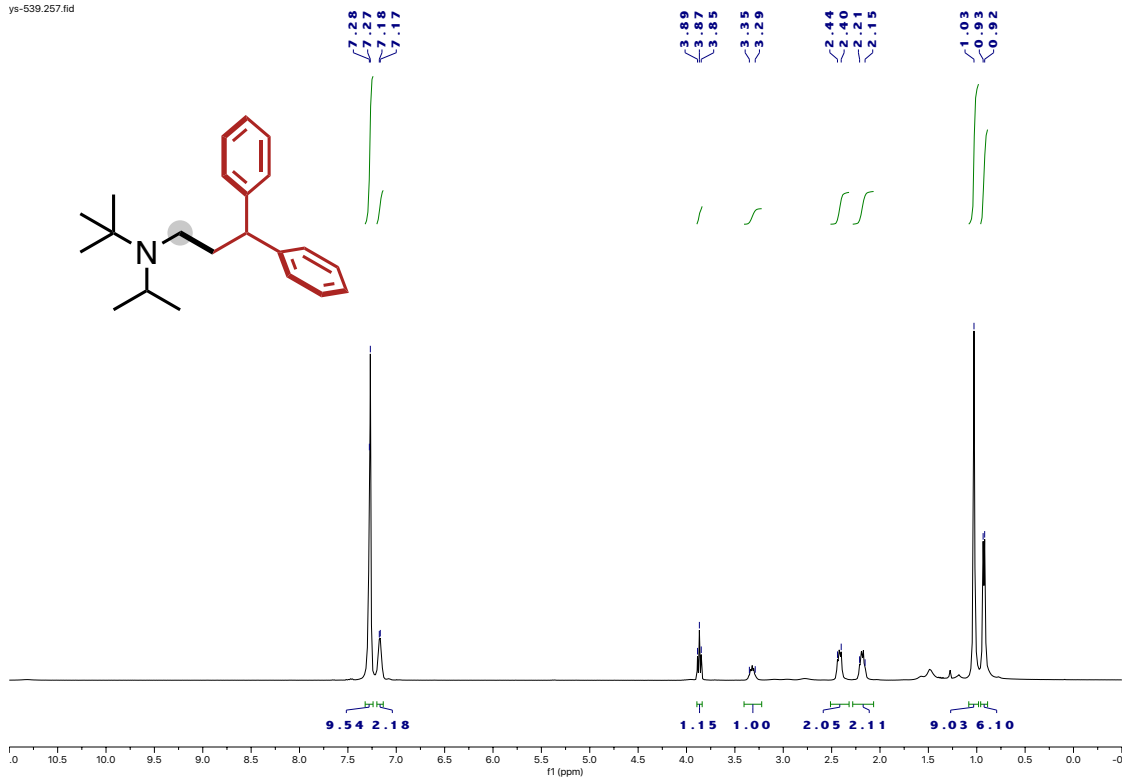
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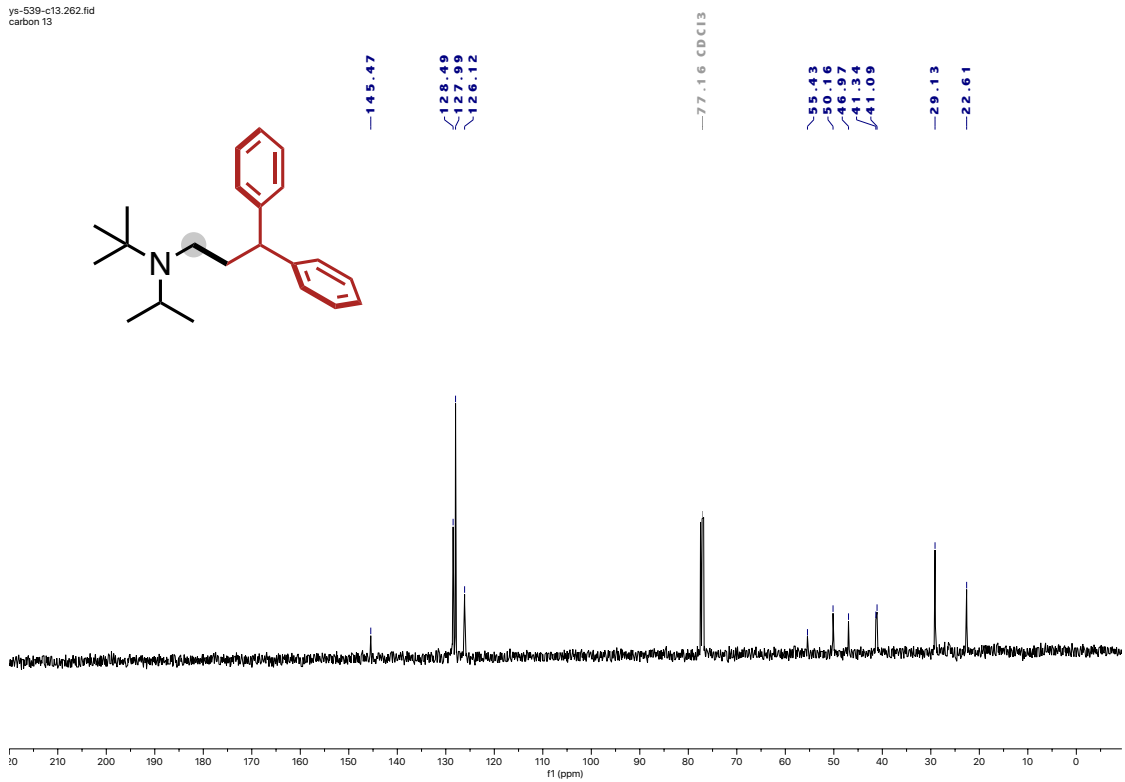
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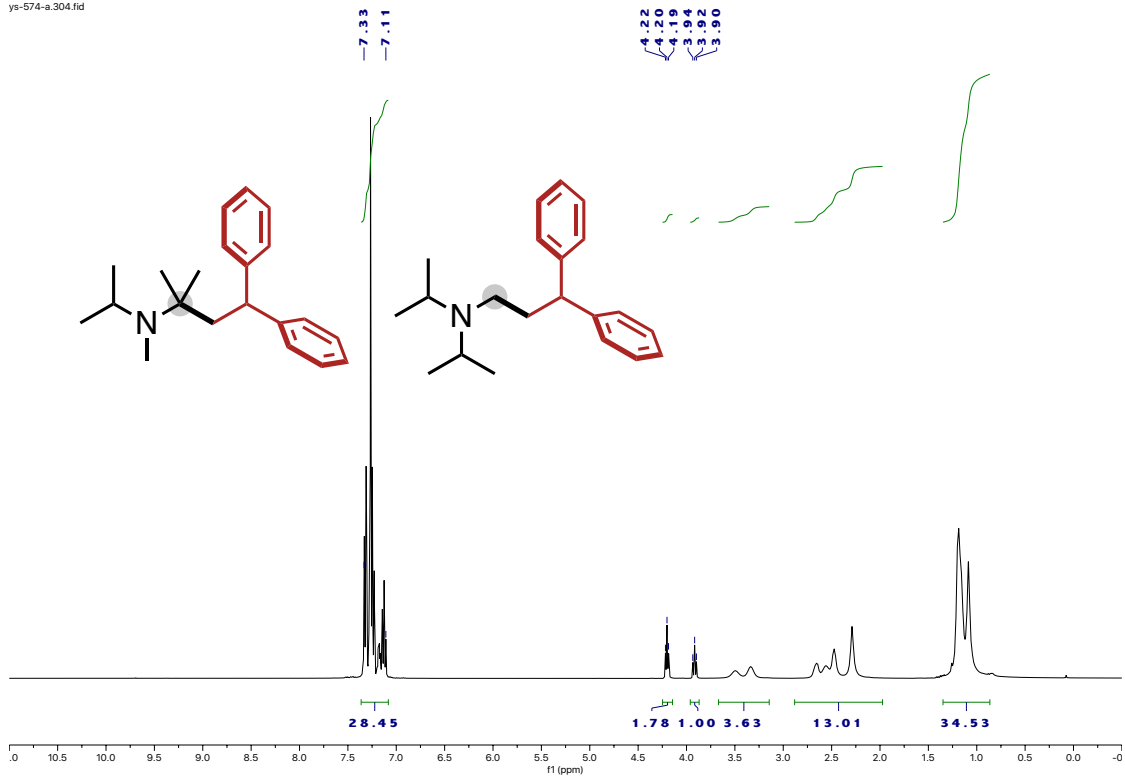
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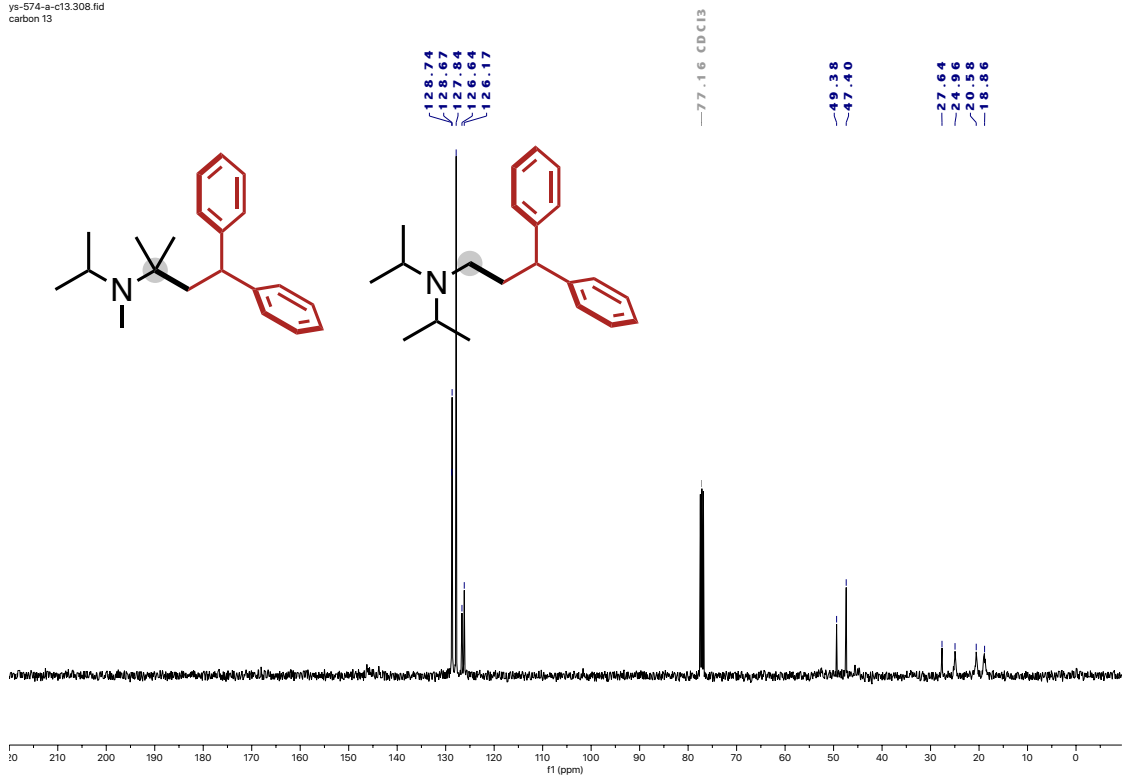
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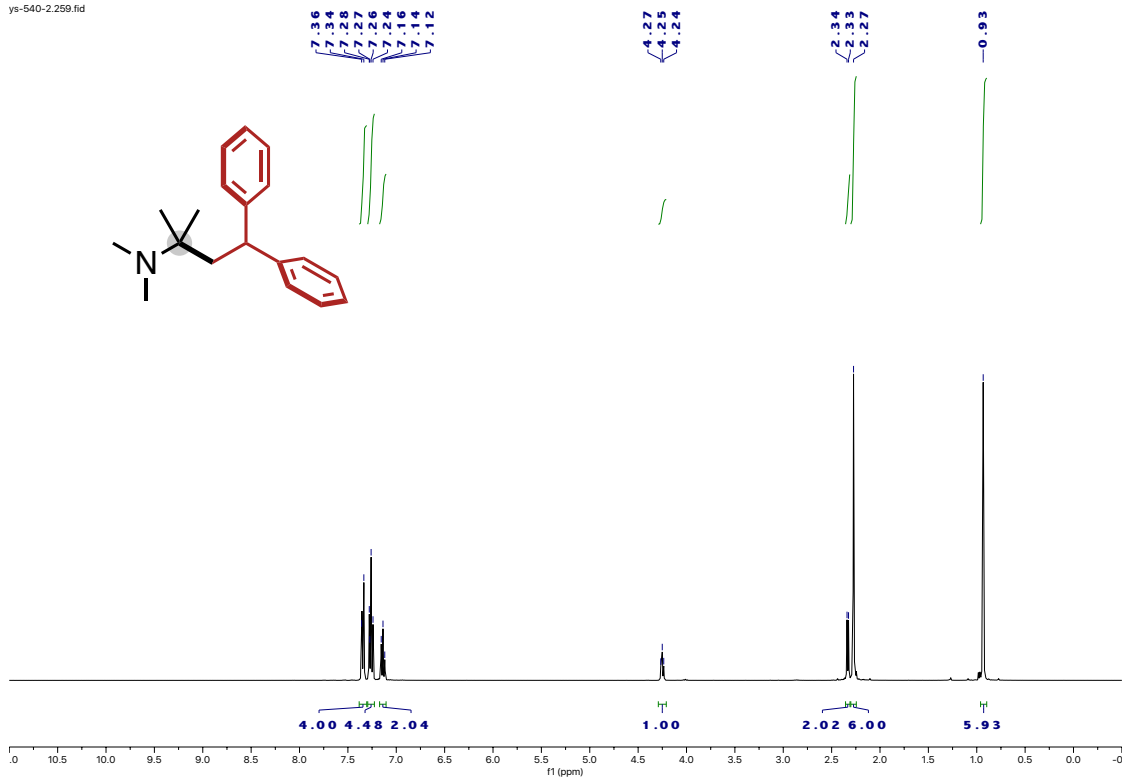
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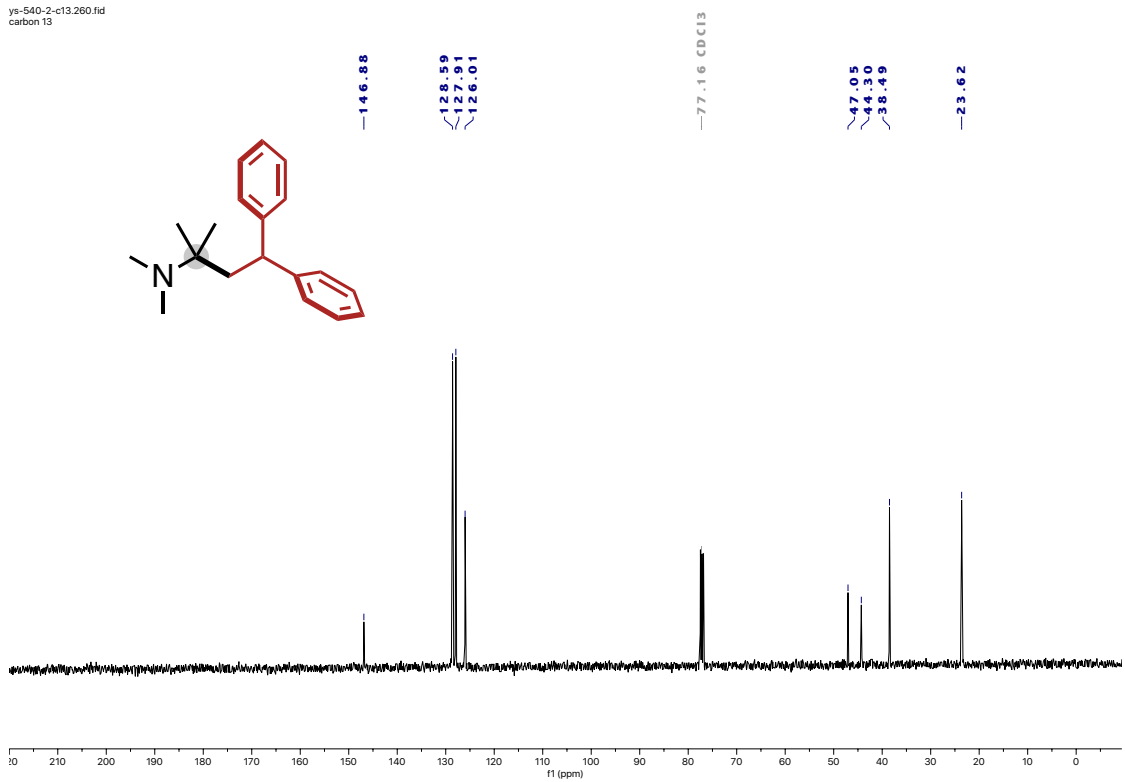
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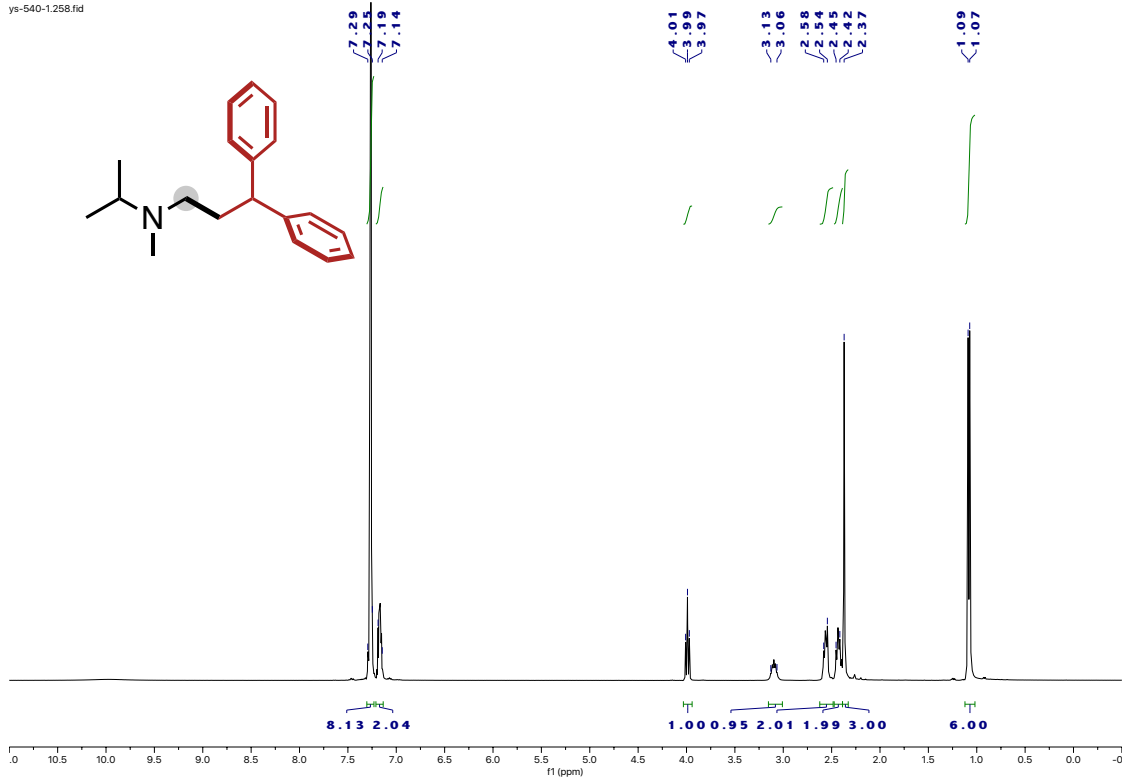
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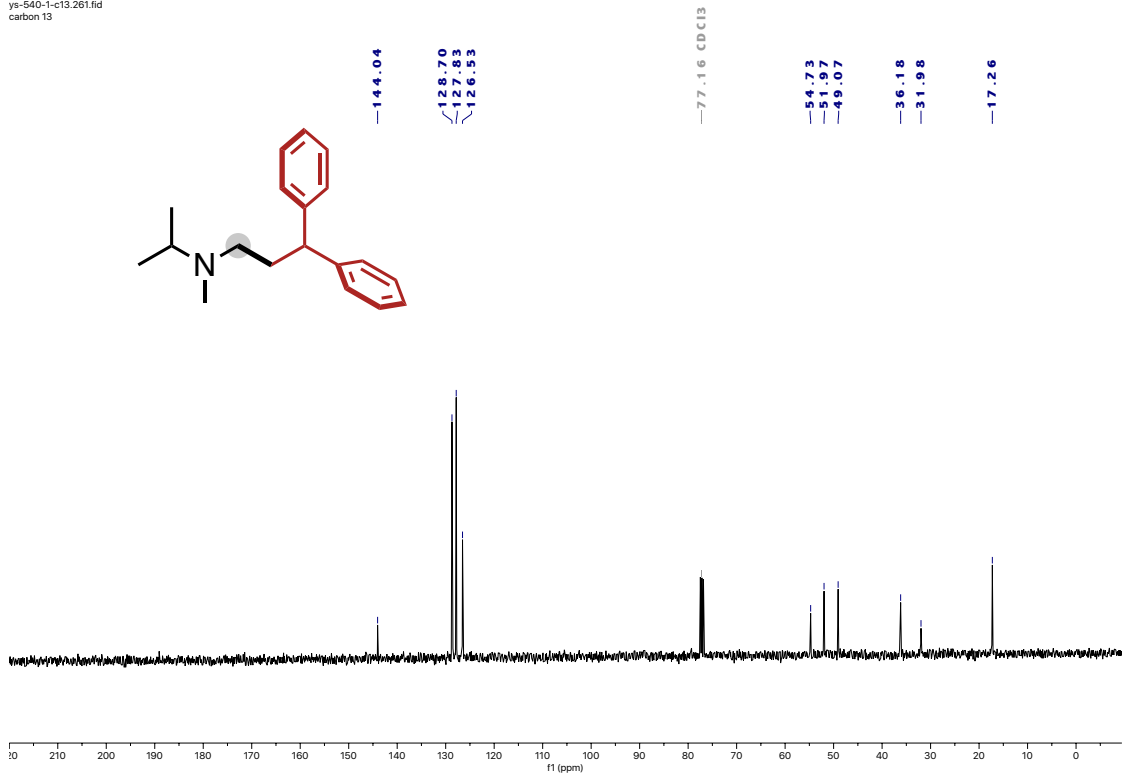
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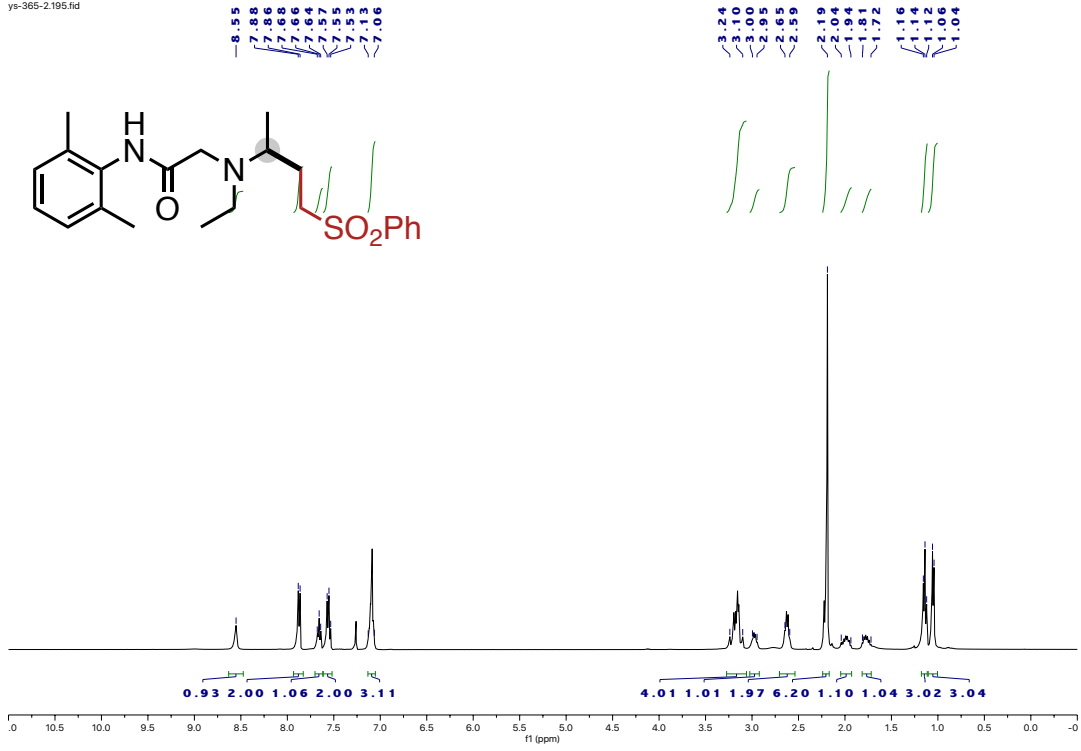
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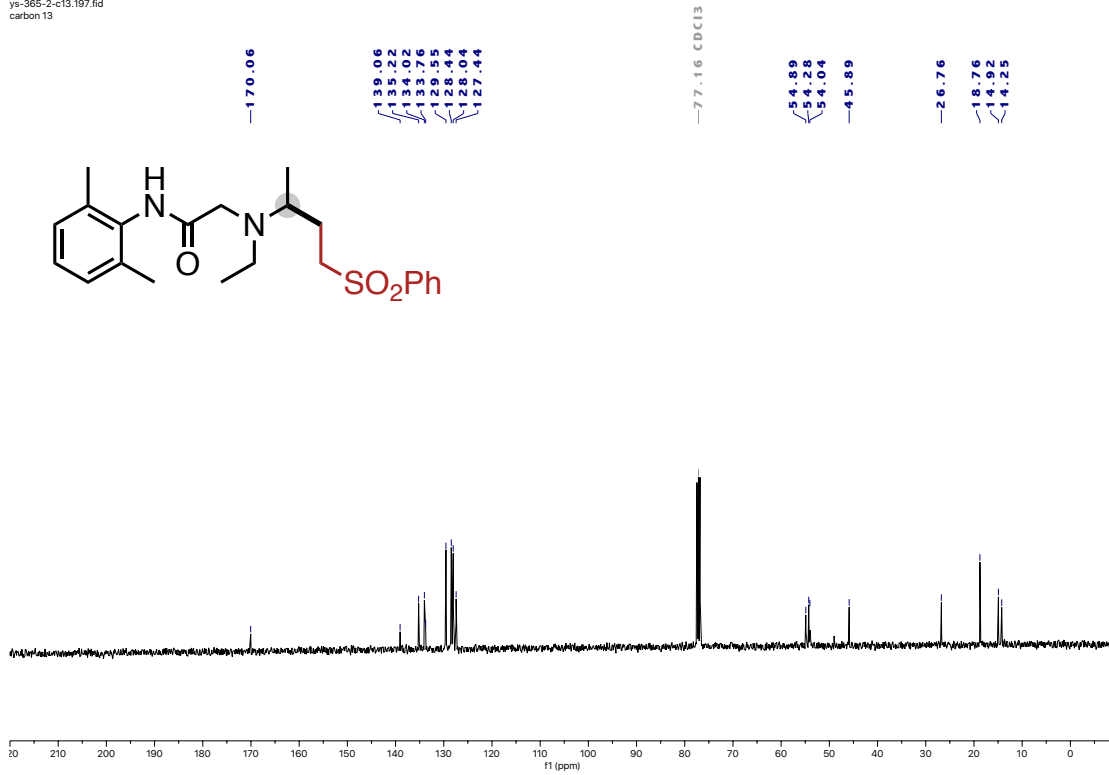
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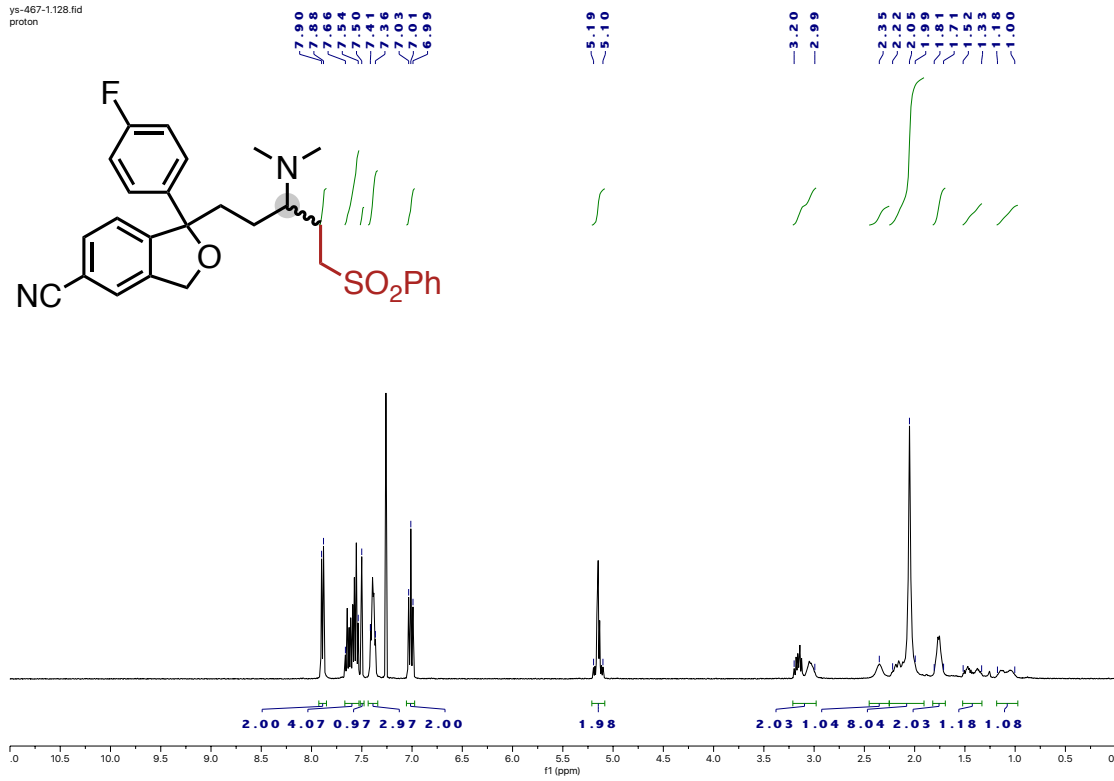
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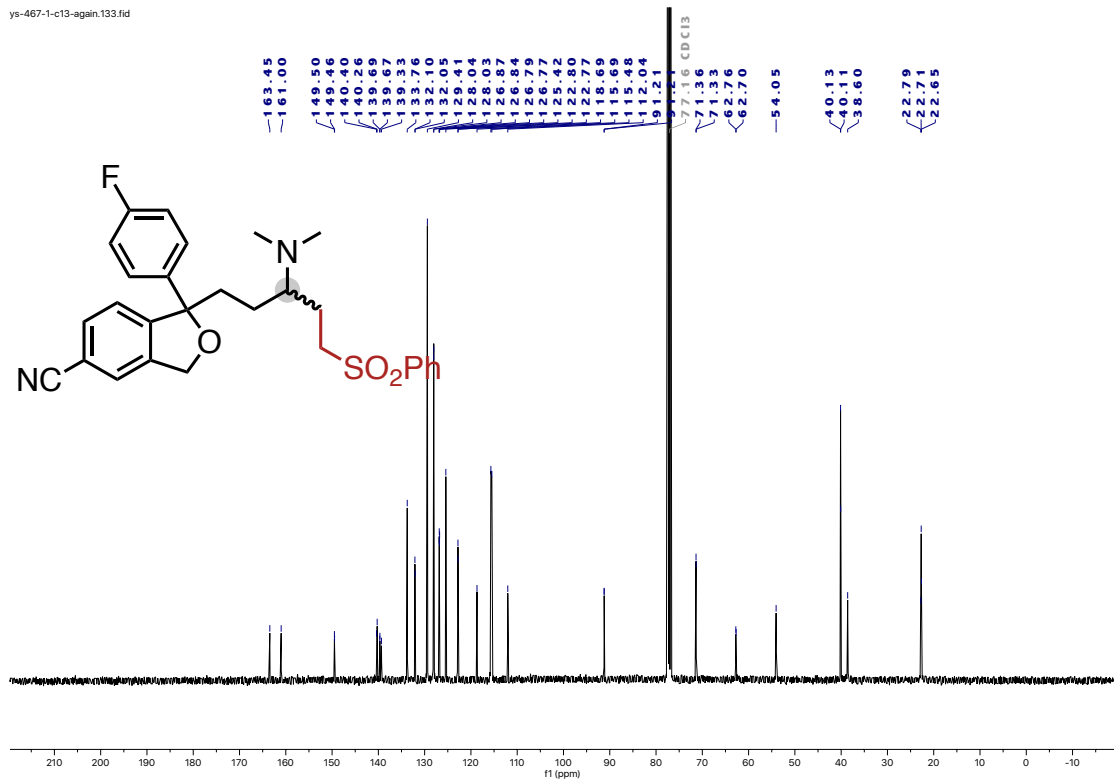
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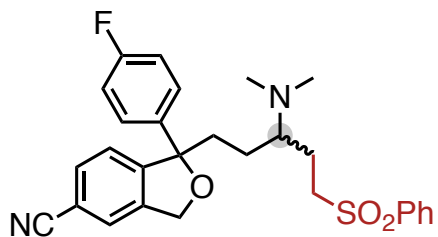
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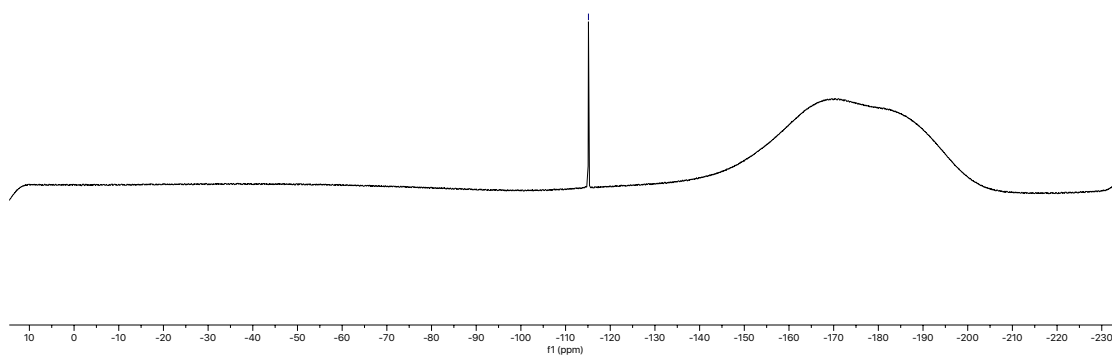
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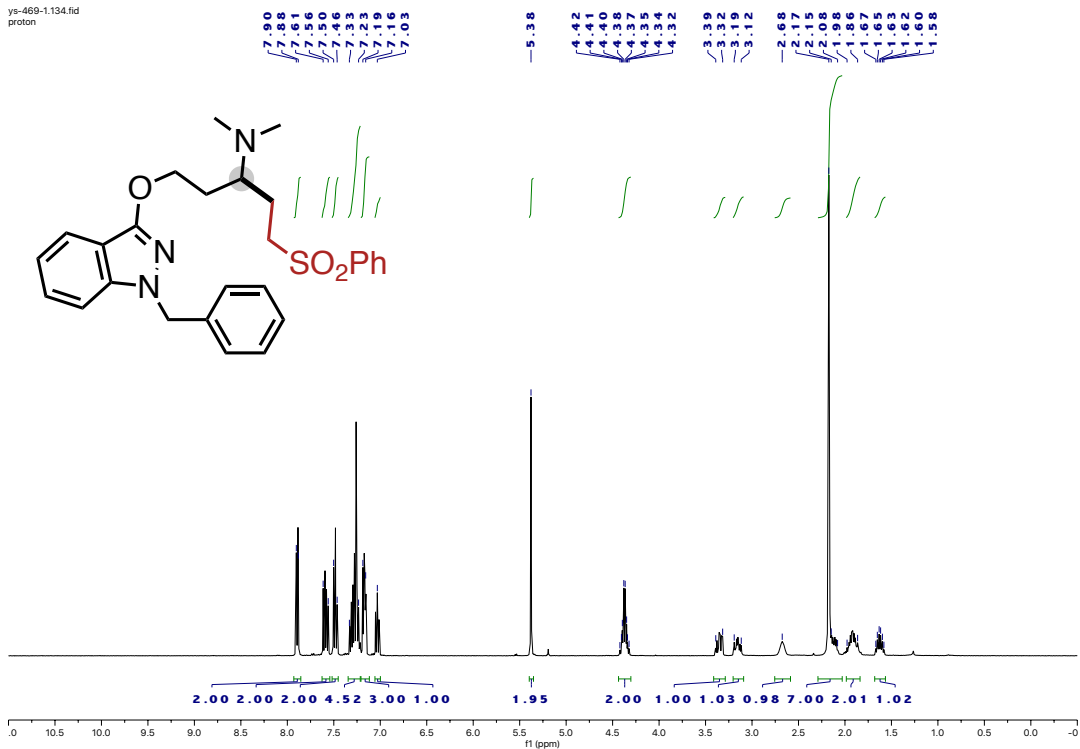
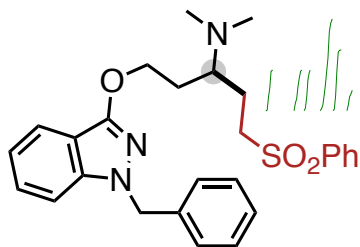
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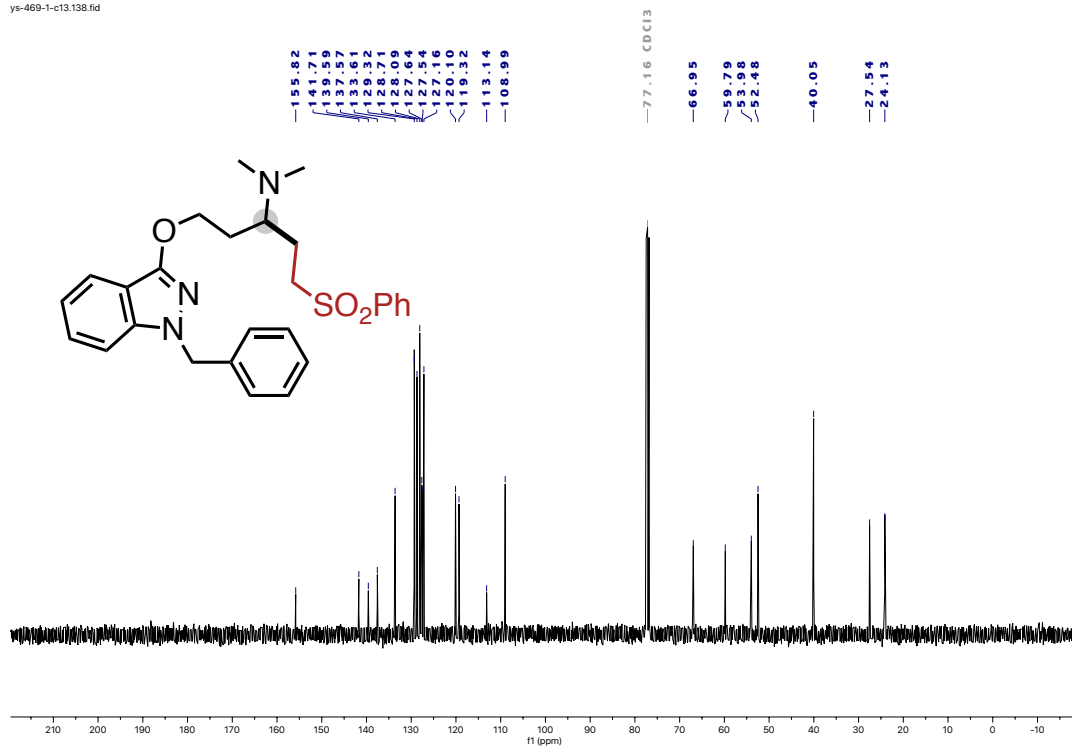
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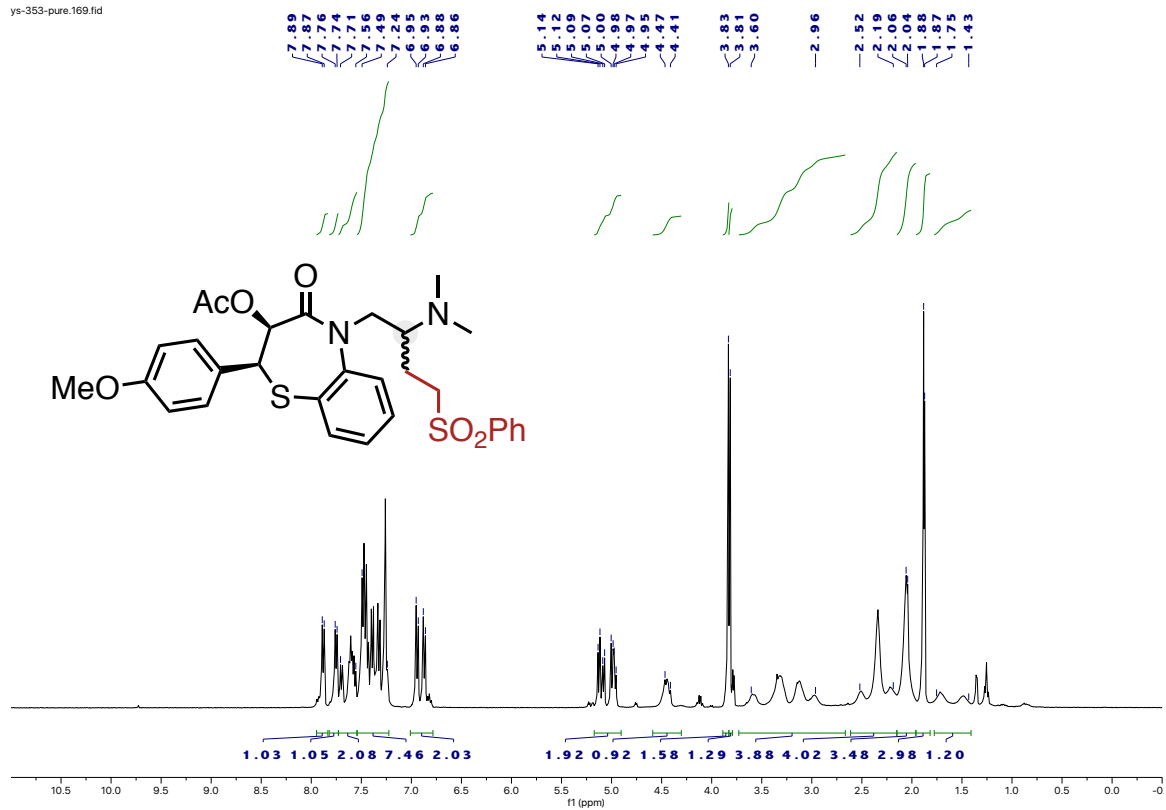
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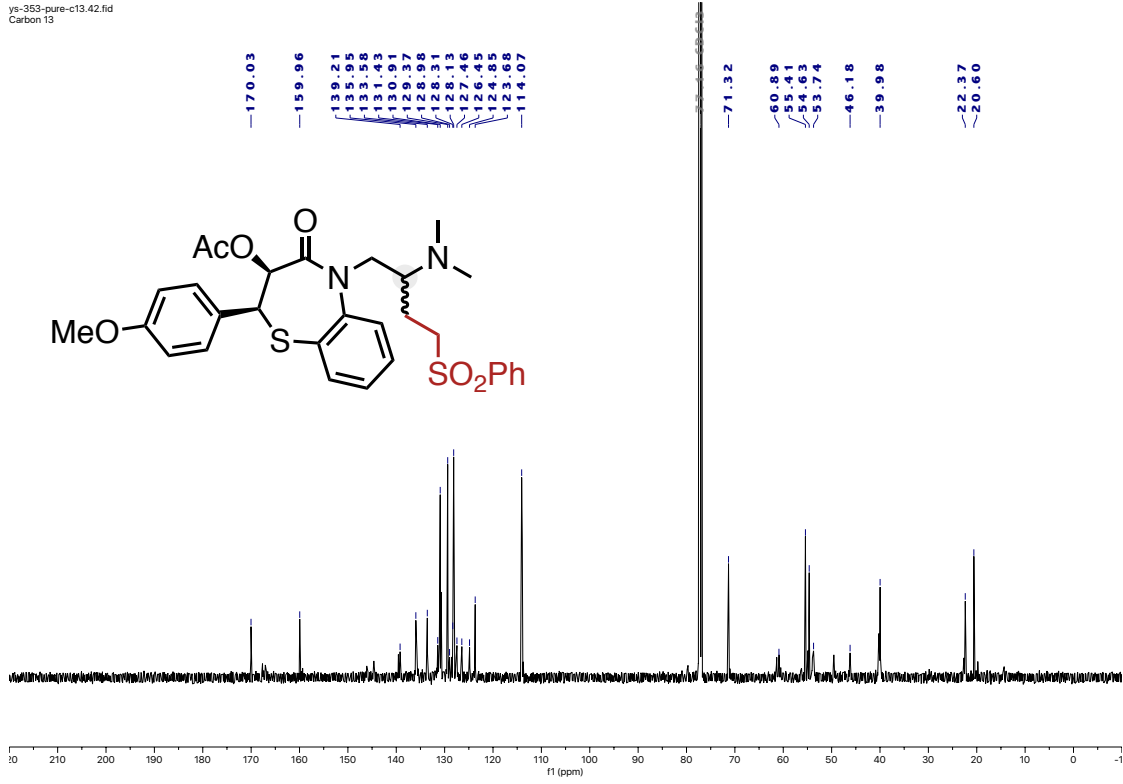
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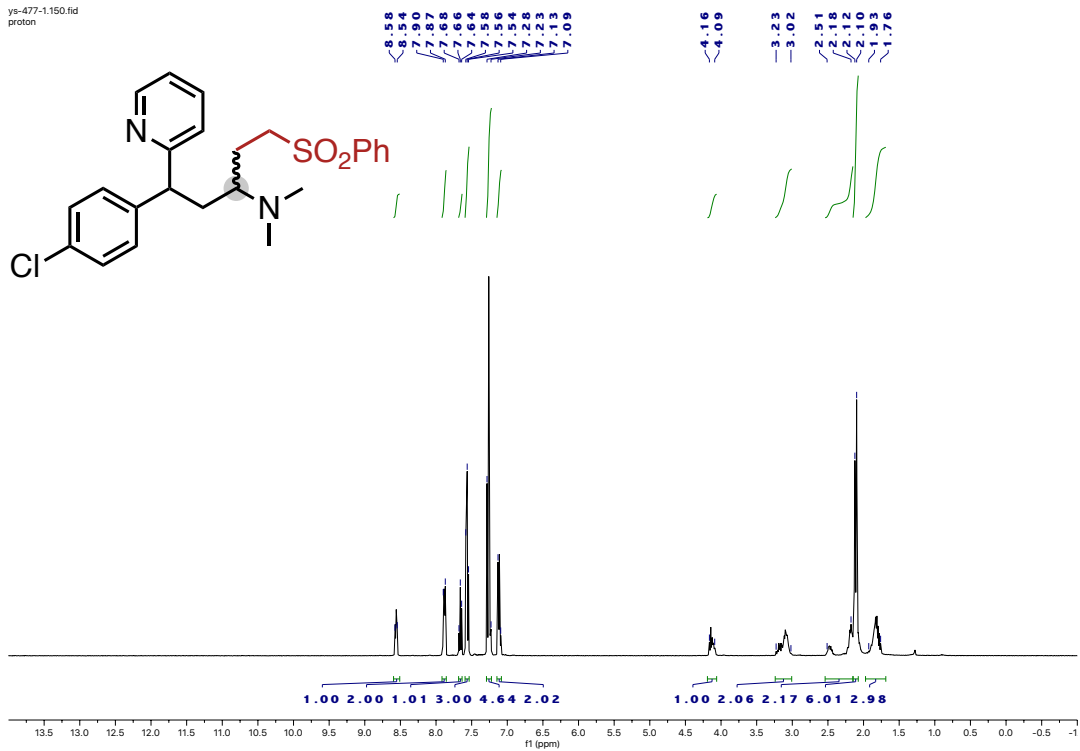
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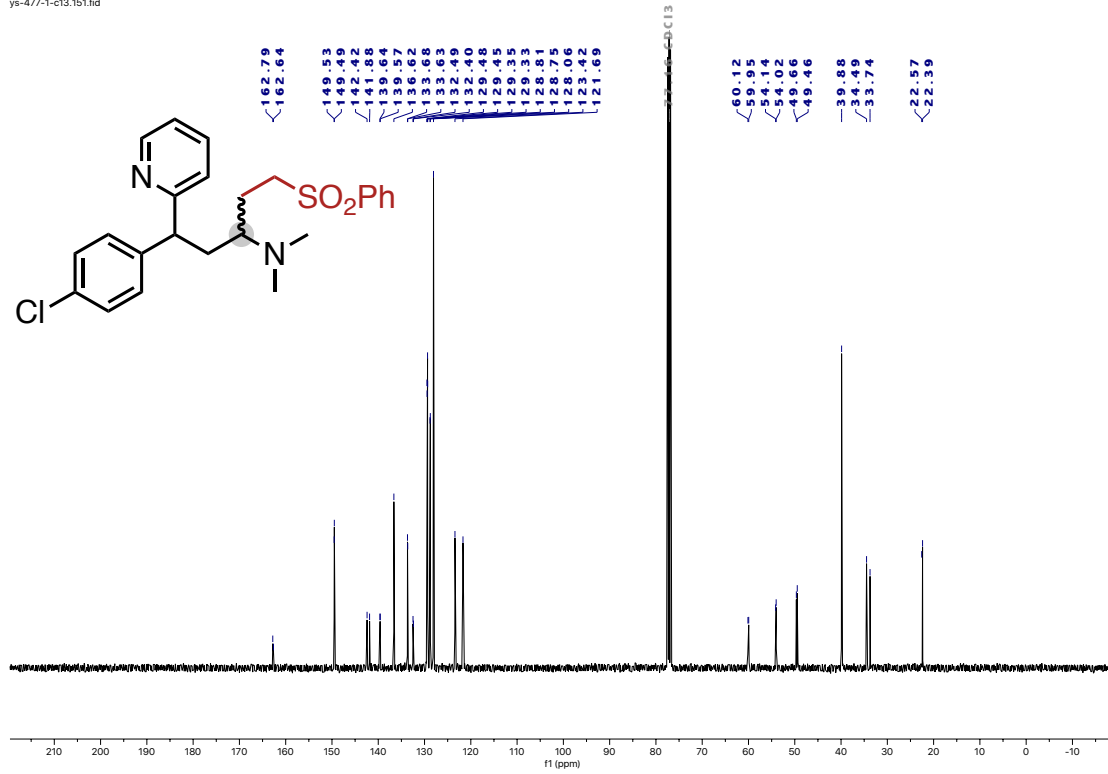
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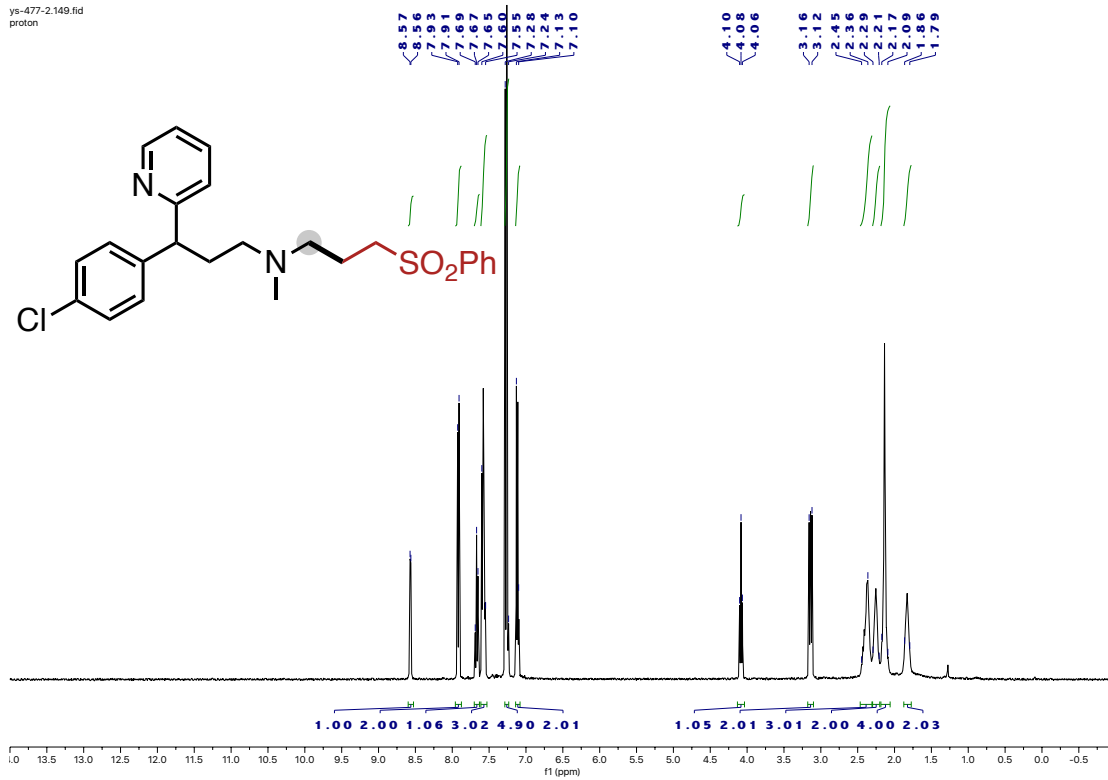
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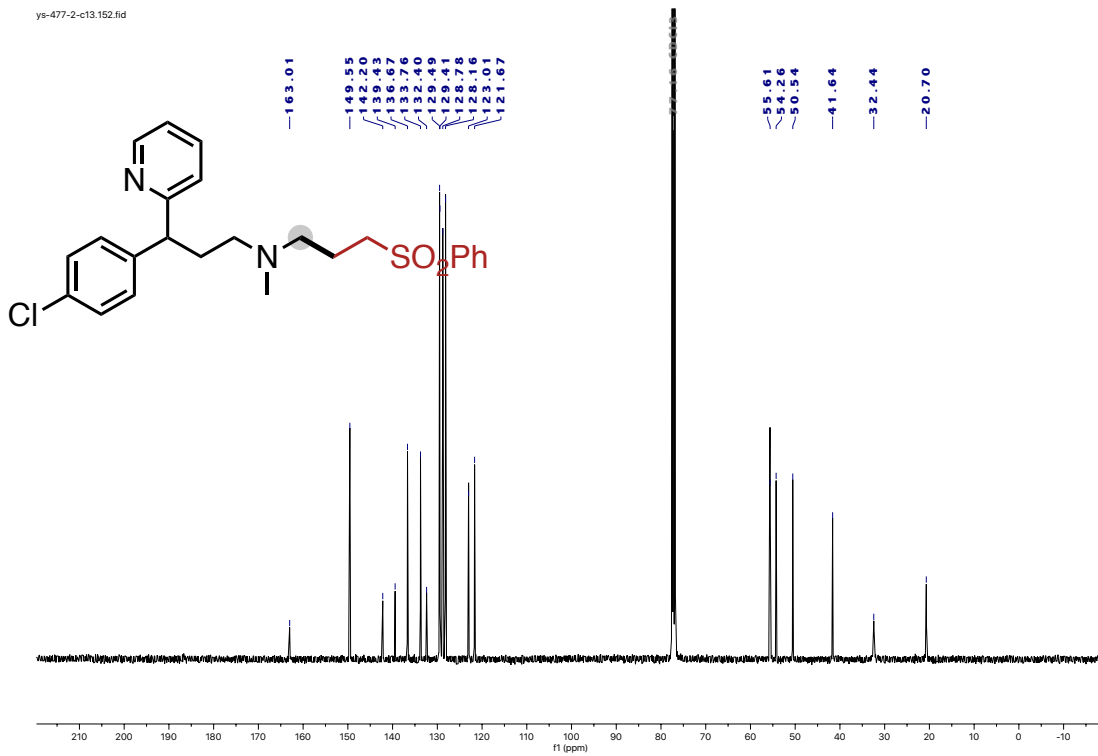
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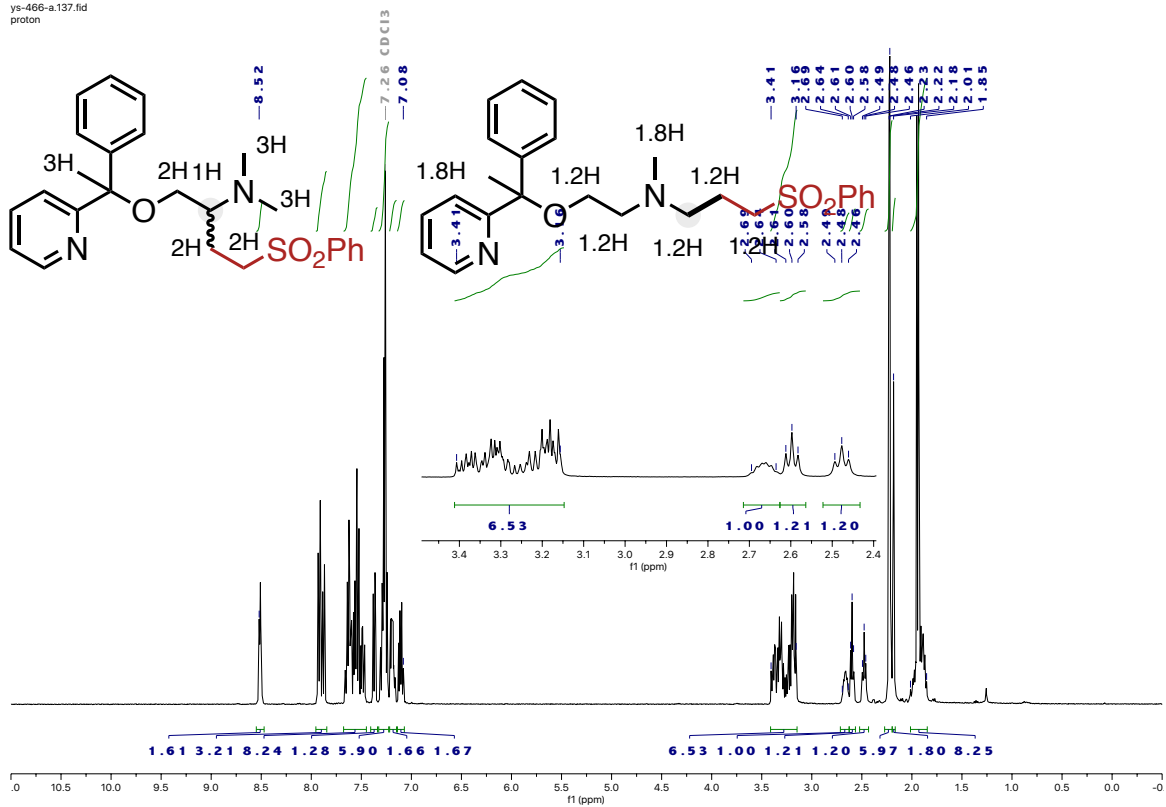
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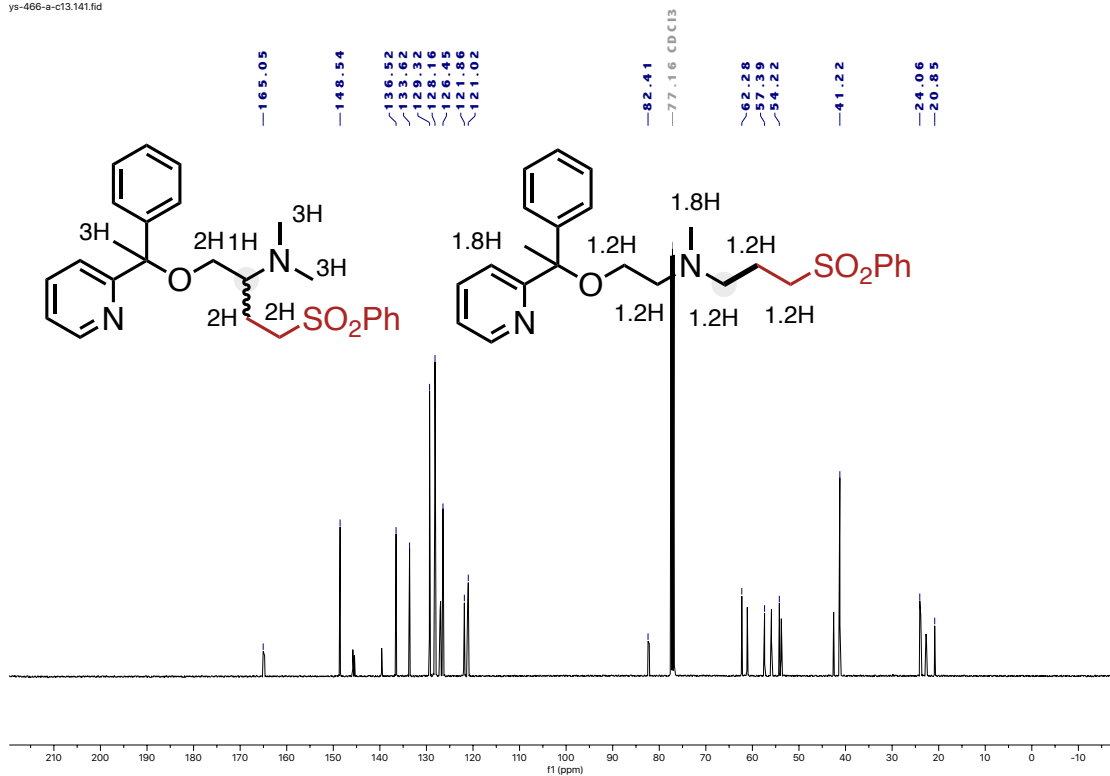
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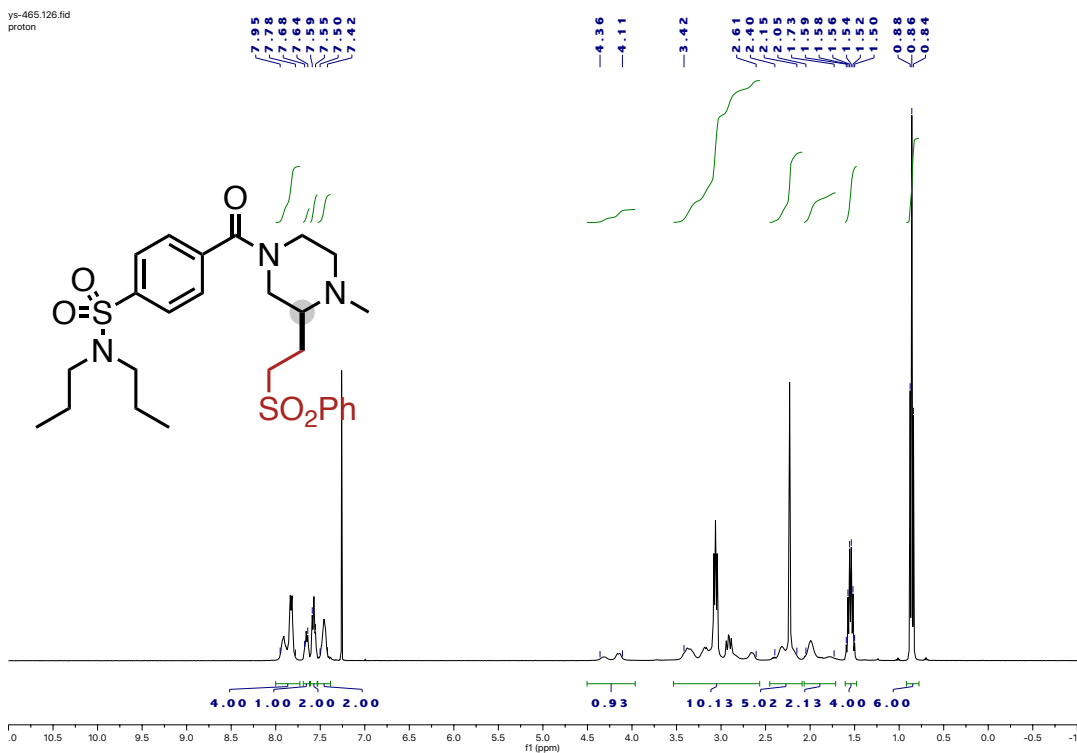
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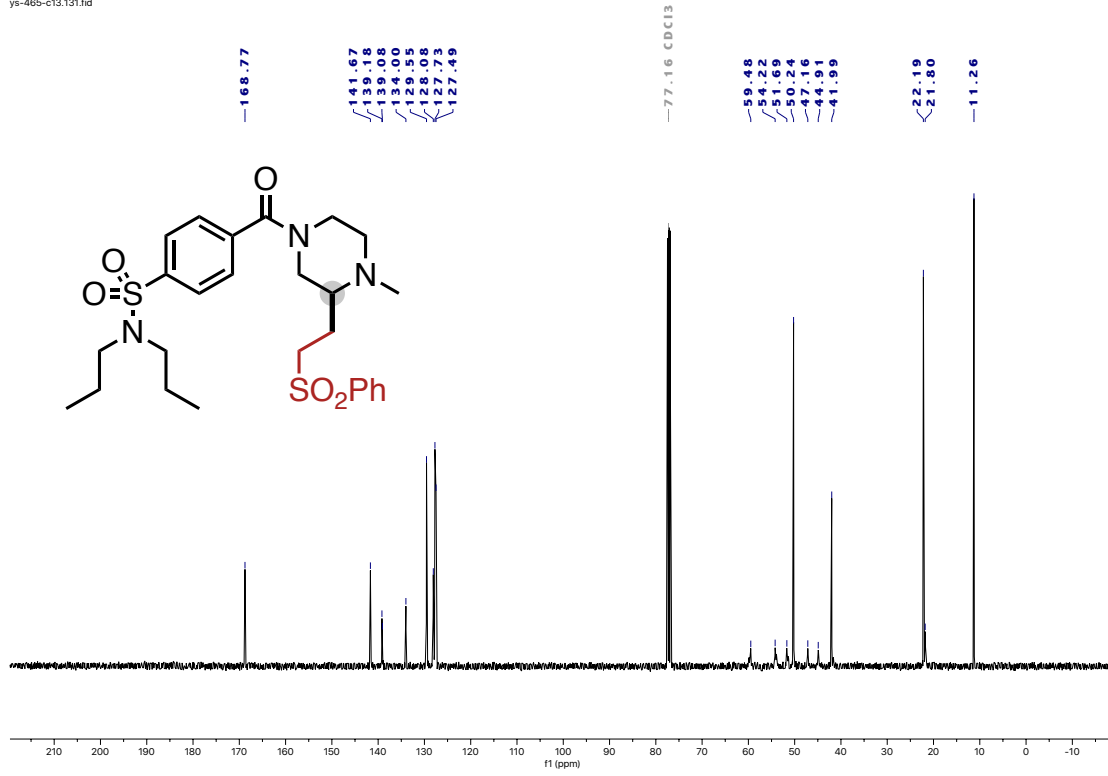
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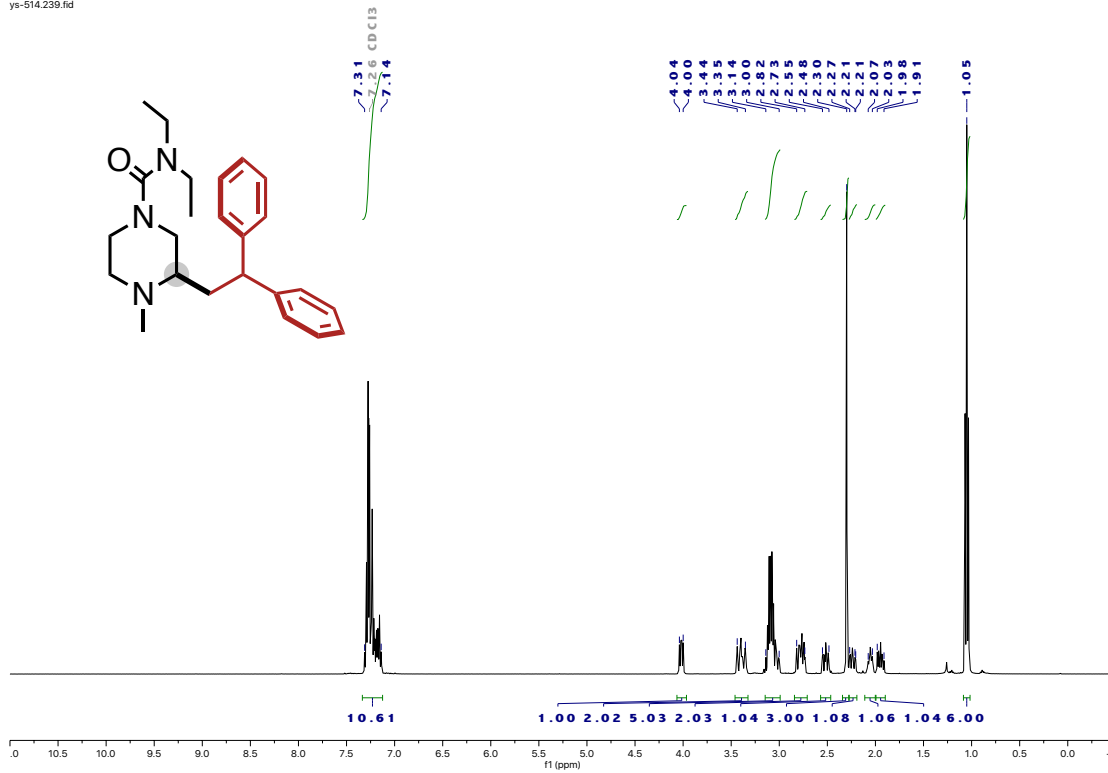
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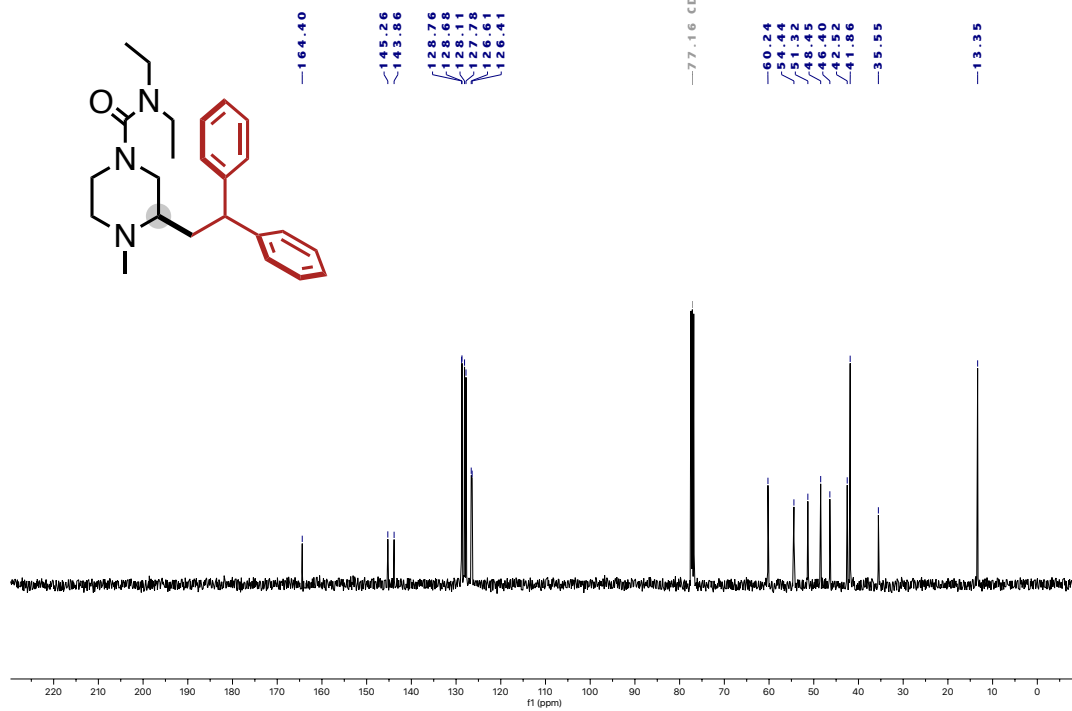
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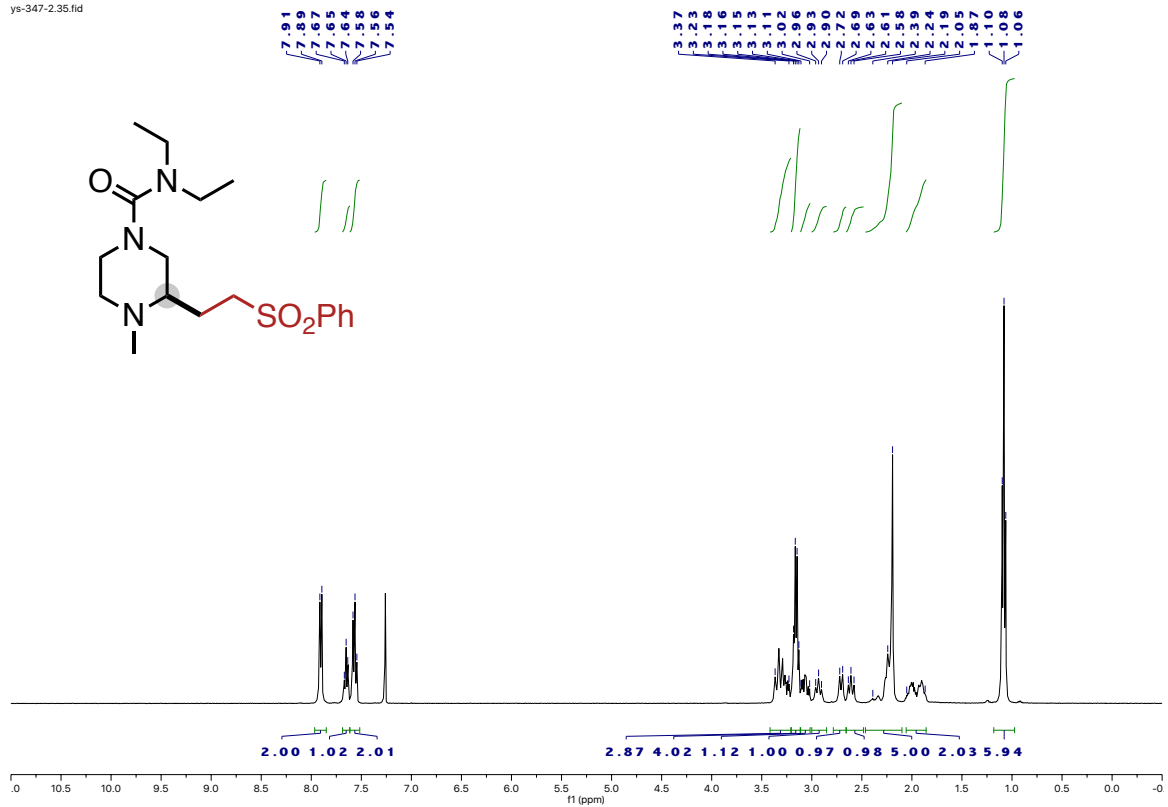
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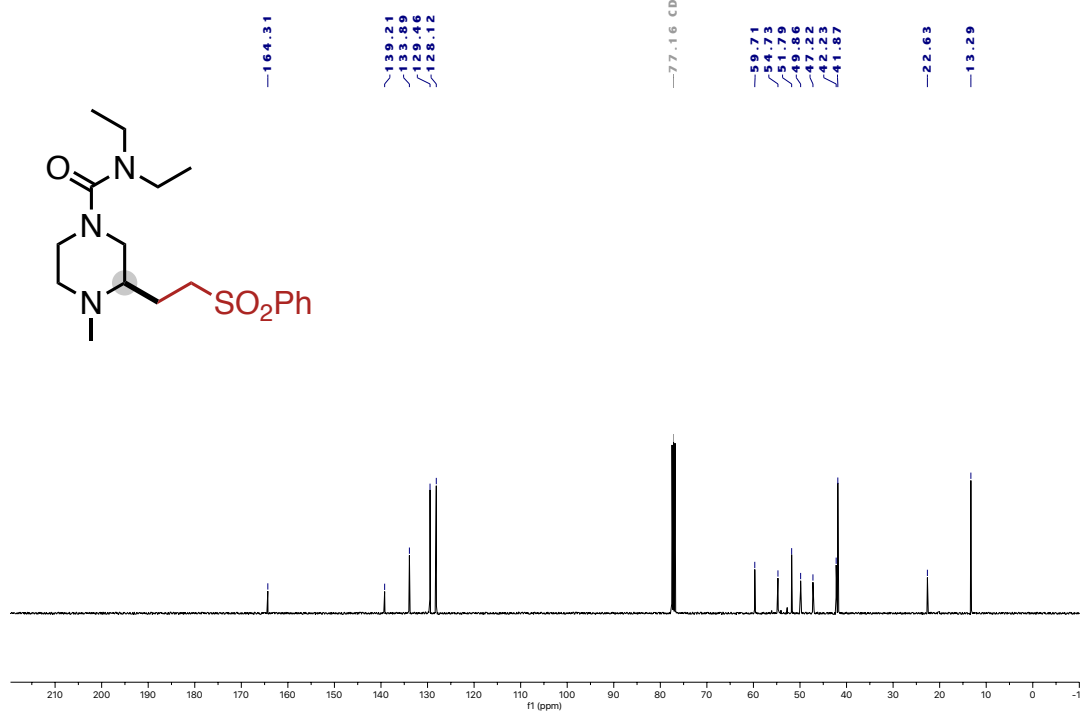
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Carbon 13



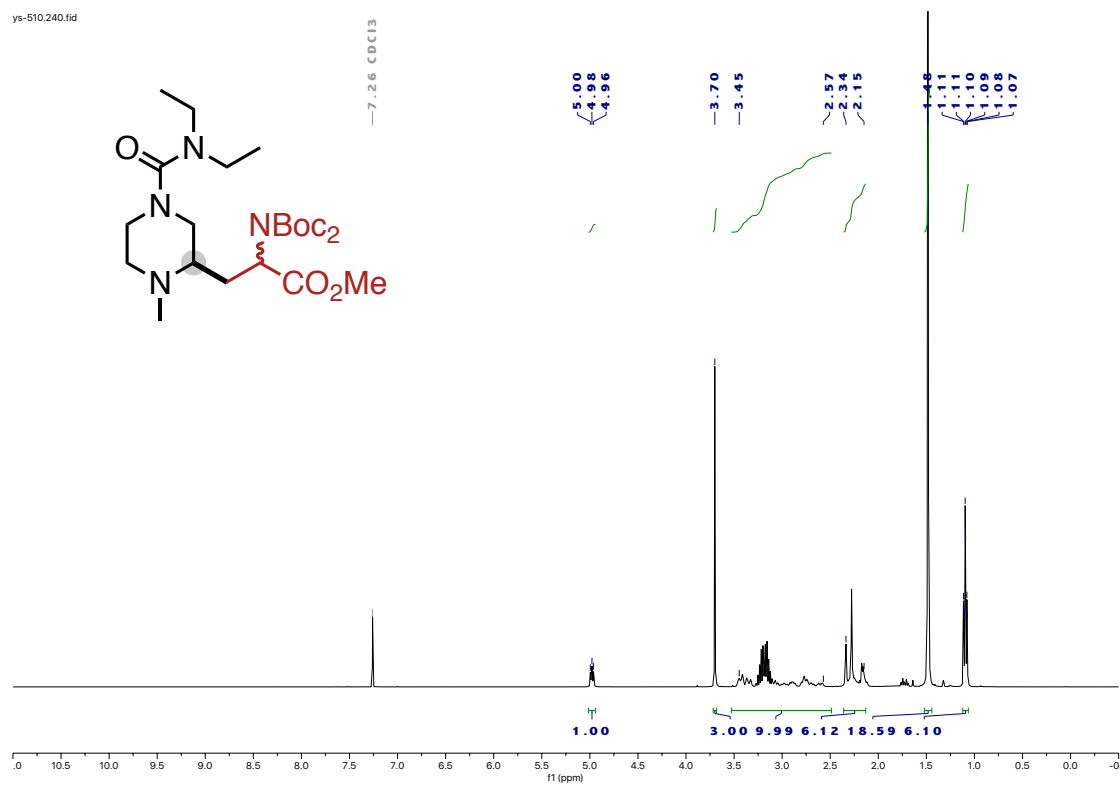
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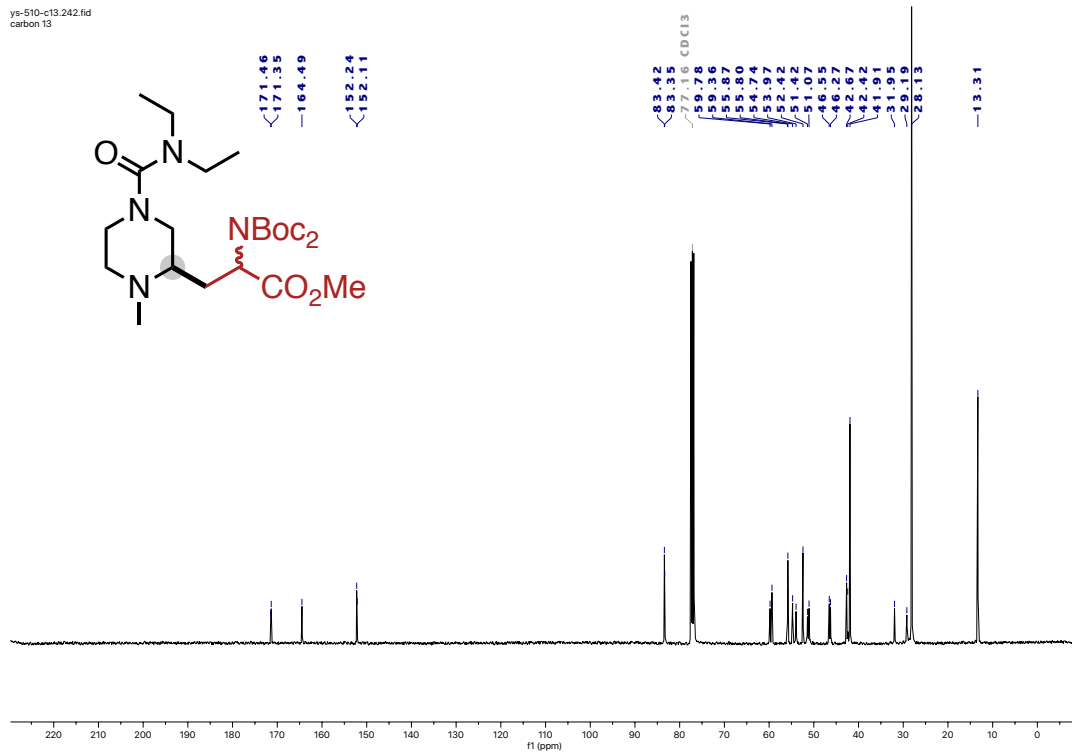
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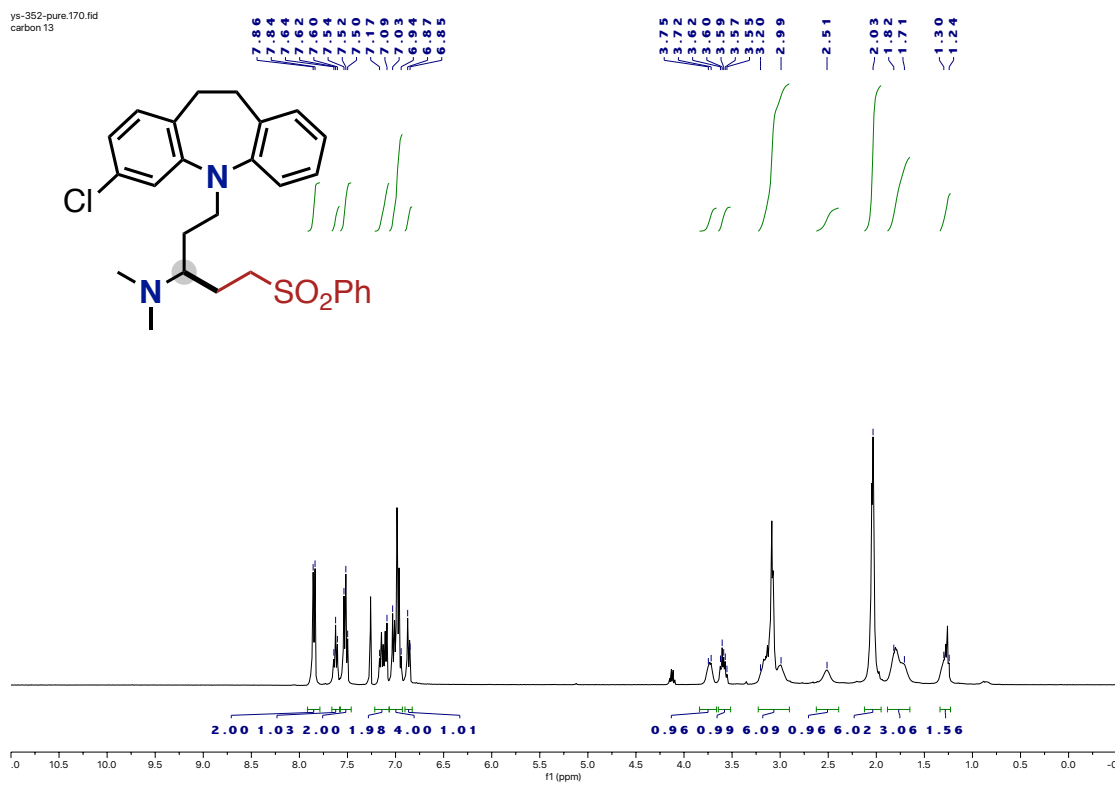
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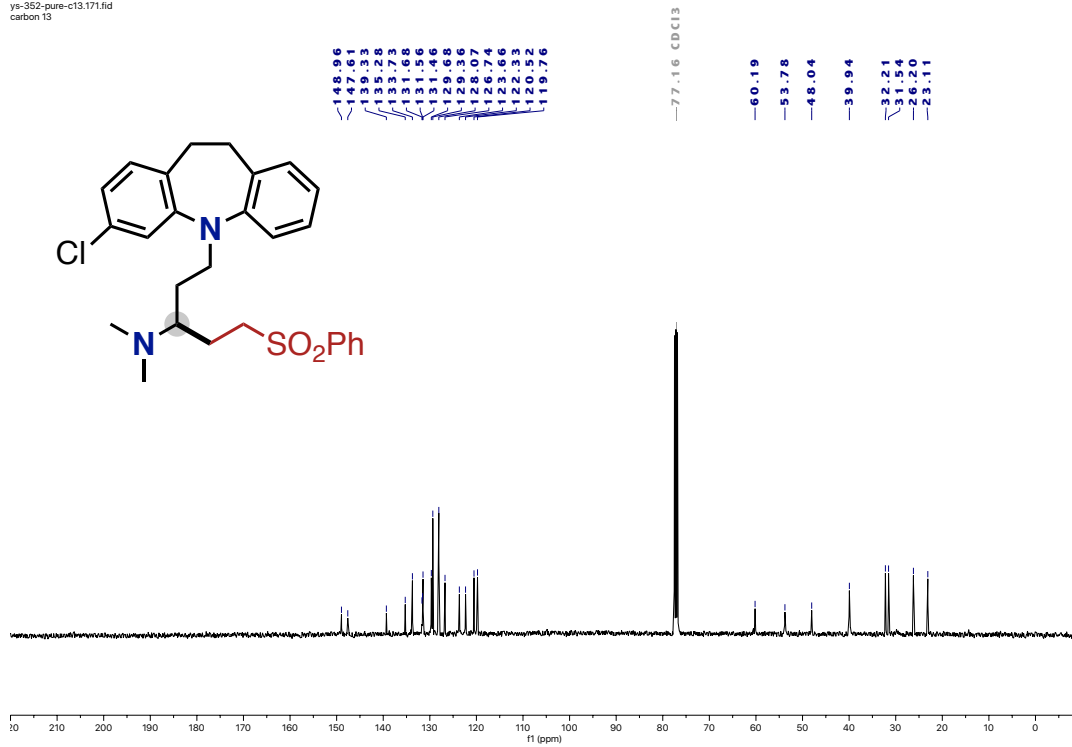
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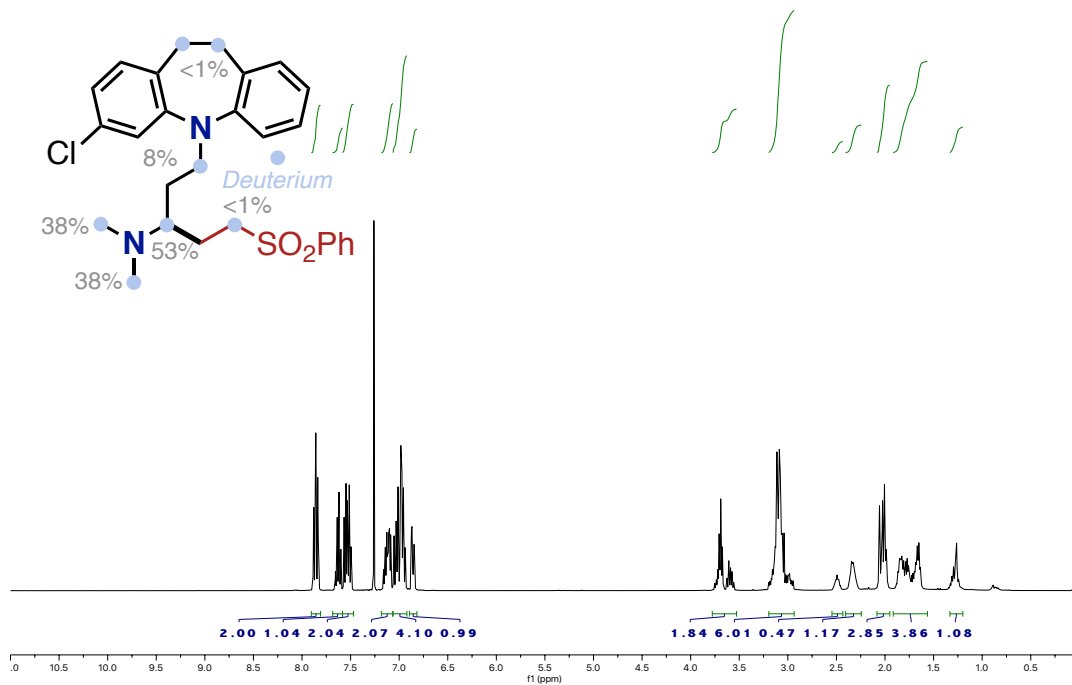
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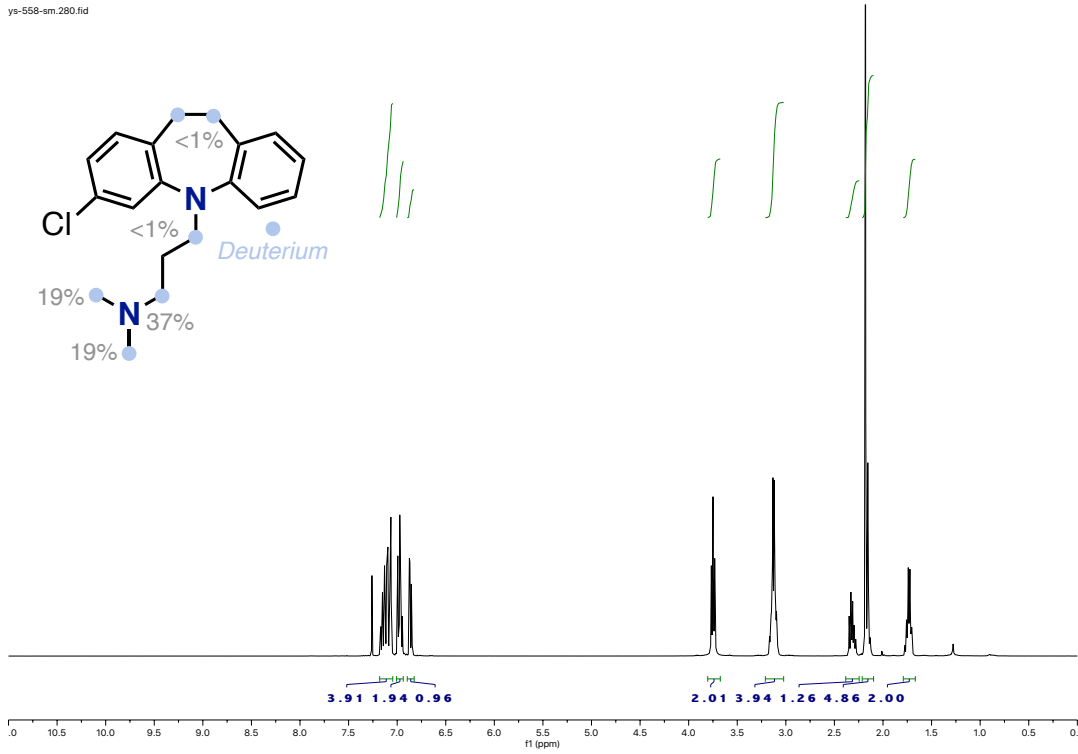
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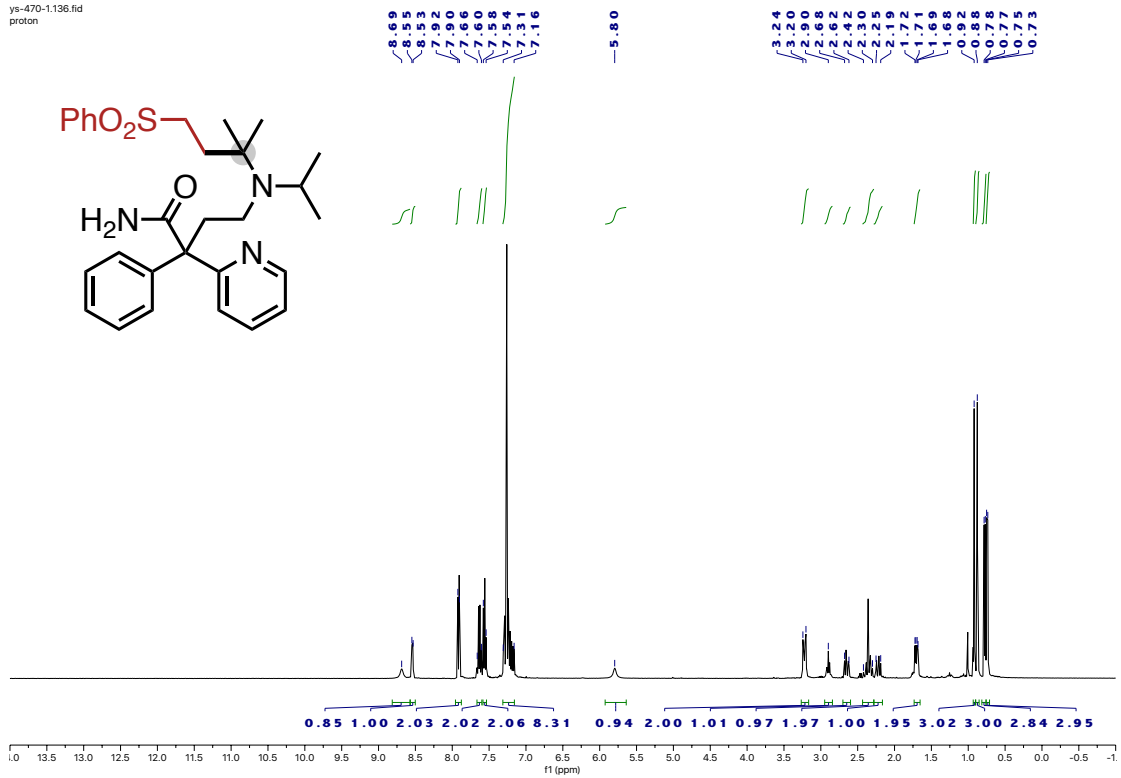
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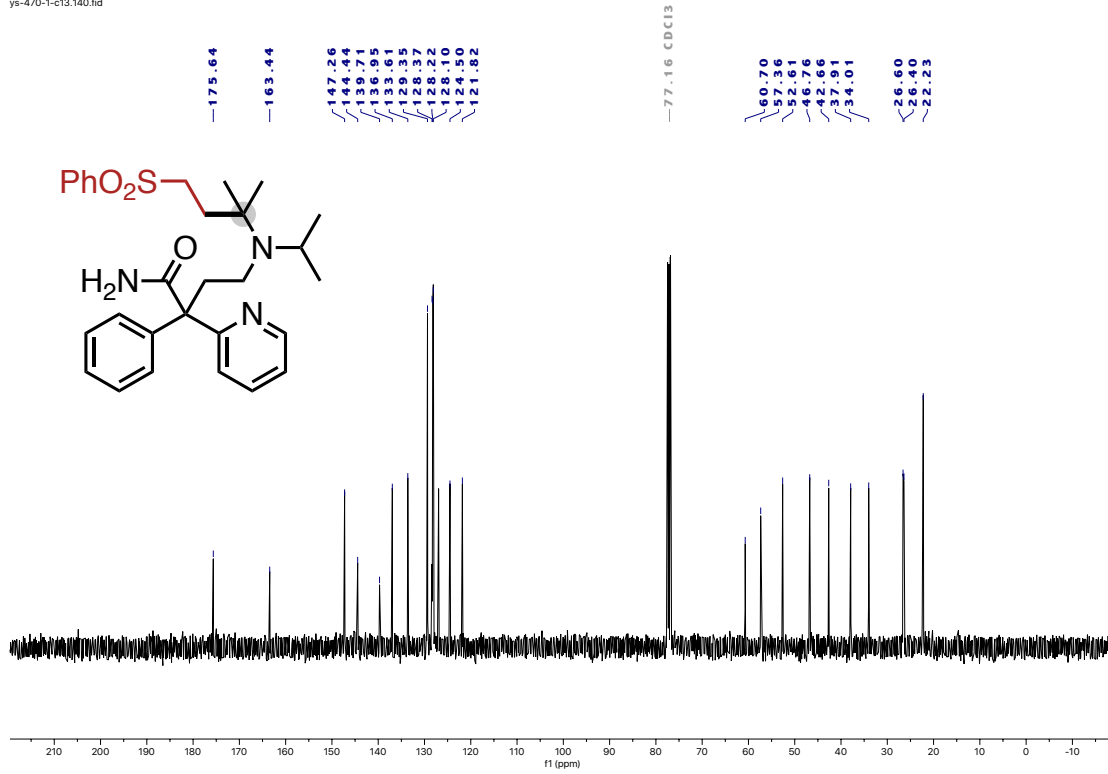
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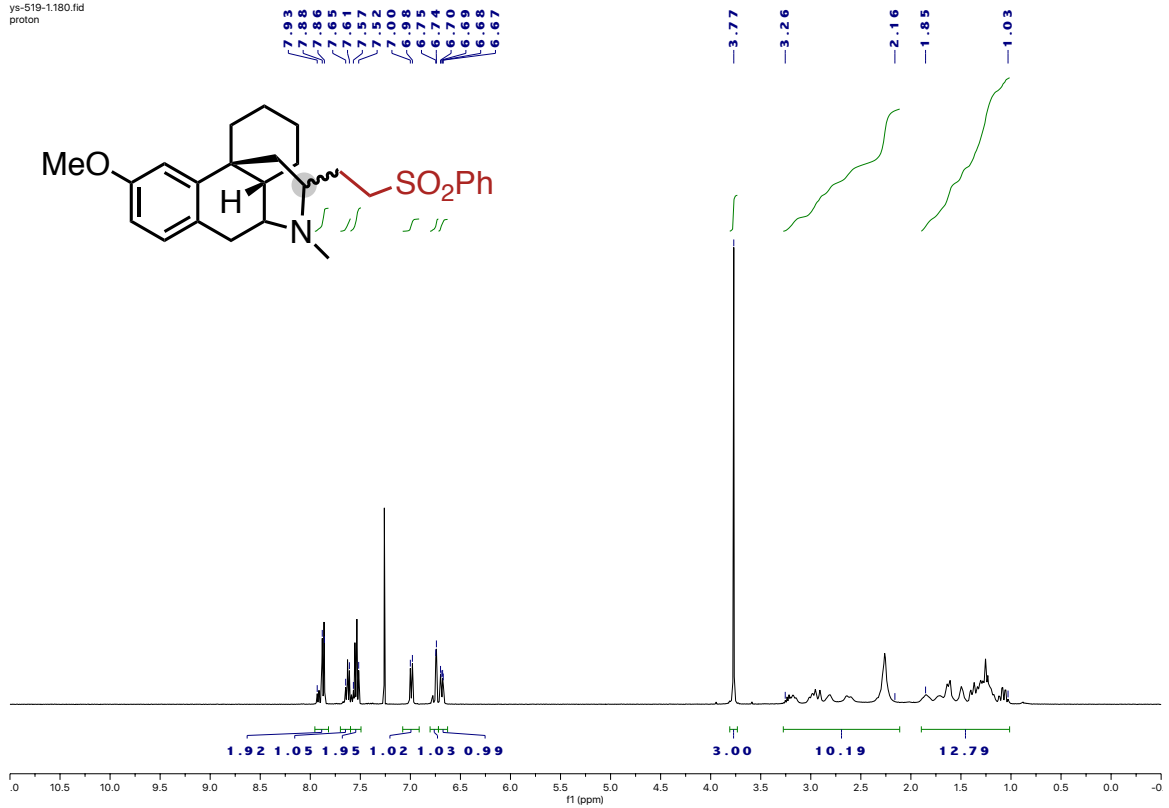
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