Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

A Catalytic Route to Dibenzodiazepines involving Buchwald-Hartwig Coupling: Reaction Scope and Mechanistic Consideration

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General procedure for the synthesis of the imine substrates

By using a Dean-Stark apparatus to facilitate water removal, $BF_3.Et_2O$ (6 mol %) was added (through a syringe) to a solution of the aldehyde and the protected amine (1 equiv.) in benzene. The mixture was heated to reflux until the theoretical quantity of water was collected. The solution was then cooled and the solvent was evaporated under vacuum to yield a solid, which was crystallized from AcOEt/Hexane (1:9) to give the desired imine product.

***N*-(2-bromobenzylidene)-4-methylbenzenesulfonamide[1] (2a):** From 2-bromobenzaldehyde (5.00g, 27mmol) and 4-methylbenzenesulfonamide, according to the general procedure the *title compound* was obtained as a white solid (7.76g, 93%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.45 (s, 3H, CH_3), 7.36 (d, *J*=8.4Hz, 2H, ArH), 7.39-7.43 (m, 2H, ArH), 7.66-7.67 (m, 1H, ArH), 7.91 (d, *J*=8.4Hz, 2H, ArH), 8.14-8.18 (m, 1H, ArH), 9.43 (br s, 1H, HC=N) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.8 (CH_3), 128.1 (CH), 128.4 (2xCH), 129.0 (C), 130.0 (2xCH), 130.8 (CH), 131.3 (C), 133.9 (CH), 134.8 (C), 135.8 (CH), 145.0 (C), 169.3 (HC=N) ppm.

***N*-(2-Bromobenzylidene)methanesulfonamide (2b):** From 2-bromobenzaldehyde (5.00g, 27mmol) and methanesulfonamide, according to the general procedure the *title compound* was obtained as a white solid (5.16g, 73%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.16 (s, 3H, CH_3), 7.44-7.49 (m, 2H, ArH), 7.67-7.71 (m, 1H, ArH), 8.19-8.21 (m, 1H, ArH), 9.47 (br s, 1H, HC=N) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 40.4 (CH_3), 128.2 (CH), 129.2 (C), 130.6 (CH), 131.1 (C), 134.1 (CH), 136.1 (CH), 171.0 (HC=N) ppm.

***N*-(2-Bromobenzylidene)-4-nitrobenzenesulfonamide[2] (2c):** From 2-bromobenzaldehyde (5.00g, 27mmol) and 4-nitrobenzenesulfonamide, according to the general procedure the *title compound* was obtained as a white solid (6.48g, 65%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.44-7.46 (m, 1H, ArH), 7.69-7.71 (m, 1H, ArH), 7.91-7.93 (m, 1H, ArH), 8.11-8.16 (m, 1H, ArH), 8.23 (d, *J*=8.4Hz, 2H, ArH), 8.40 d, *J*=8.4Hz, 2H, ArH), 9.56 (br s, 1H, HC=N) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 124.6 (2xCH), 128.1 (C), 128.3 (CH), 129.7 (2xCH), 130.9 (CH), 134.2 (CH), 135.5 (C), 136.7 (CH), 144.0 (C), 150.9 (C), 171.6 (HC=N) ppm.

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[1] Ma, G. N; Zhang, T.; Shi, M.; *Org Lett*, **2009**, *11*, 875-878
[2] R. A. Brawn, J. S. Panek, *Org. Lett.* **2009**, *11*, 4362-4363

***N*-(2-bromo-5-fluorobenzylidene)-4-methylbenzenesulfonamide[3] (2d):** From 2-bromo-5-fluorobenzaldehyde (1.00g, 4.9mmol) and 4-methylbenzenesulfonamide, according to the general procedure the *title compound* was obtained as a white solid (1.42g, 81%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.45 (s, 3H, CH_3), 7.15-7.20 (m, 1H, ArH), 7.37 (d, *J*=8.8Hz, 2H, ArH), 7.61-7.65 (m, 1H, ArH), 7.82-7.85 (m, 1H, ArH), 7.89 (d, *J*=8.8Hz, 2H, ArH), 9.36 (d, *J*=2.0Hz, 1H, HC=N) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.8 (CH_3), 117.0 (d, *J*=24.1Hz, CH), 123.0 (C), 123.1 (d, *J*=22.9Hz, CH), 128.4 (2xCH), 130.0 (2xCH), 132.9 (d, *J*=7.5Hz, C), 134.4 (C), 135.2 (d, *J*=7.4Hz, CH), 145.2 (C), 161.9 (d, *J*=248.6Hz, C-F), 168.0 (d, *J*=2.2Hz, HC=N) ppm.

***N*-(2-Bromo-5-methoxybenzylidene)-4-methylbenzenesulfonamide[3] (2e):** From 2-bromo-5-methoxybenzaldehyde (1.00g, 4.7mmol) and 4-methylbenzenesulfonamide, according to the general procedure the *title compound* was obtained as a white solid (1.25g, 72%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.44 (s, 3H, CH_3), 3.87 (s, 3H, OMe), 6.87-6.90 (m, 1H, ArH), 7.15 (d, *J*=2.4Hz, 1H, ArH), 7.34 (d, *J*=8.0Hz, 2H, ArH), 7.88 (d, *J*=8.0Hz, 2H, ArH), 8.12 (d, *J*=8.8Hz, 1H, ArH) 9.33 (br s, 1H, HC=N) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.8 (CH_3), 56.1 (OMe), 114.7 (CH), 118.7 (CH), 124.1 (C), 128.3 (2xCH), 129.9 (2xCH), 130.9 (C), 132.3 (2xCH), 135.5 (C), 144.6 (C), 165.3 (C), 168.6 (HC=N) ppm.

***N*-(2-Bromo-4-methoxybenzylidene)-4-methylbenzenesulfonamide[3] (2f):** From 2-bromo-4-methoxybenzaldehyde (1.00g, 4.7mmol) and 4-methylbenzenesulfonamide, according to the general procedure the *title compound* was obtained as a white solid (1.28g, 75%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.45 (s, 3H, CH_3), 3.81 (s, 3H, OMe), 7.00-7.03 (m, 1H, ArH), 7.36 (d, *J*=8.4Hz, 2H, ArH), 7.52 (d, *J*=8.8Hz, 1H, ArH), 7.62 (d, *J*=3.2Hz, 1H, ArH), 7.90 (d, *J*=8.4Hz, 2H, ArH), 9.36 (br s, 1H, HC=N) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.8 (CH_3), 56.0 (OMe), 113.5 (CH), 120.0 (C), 123.9 (CH), 128.5 (2xCH), 130.0 (2xCH), 131.8 (C), 134.6 (CH), 134.7 (C), 145.0 (C), 159.3 (C), 169.4 (HC=N) ppm.

***N*-(2-Bromo-5-hydroxy-4-methoxybenzylidene)-4-methylbenzenesulfonamide (2g):** From 2-bromo-5-hydroxy-4-methoxybenzaldehyde (1.00g, 0.0043mol) and 2-bromo-5-

[3] M. Fujioka, T. Morimoto, T. Tsumagari, H. Tanimoto, Y. Nishiyama, K. Kakiuchi, *J. Org. Chem*. **2012**, *77*, 2911-2923.

hydroxy-4-methoxybenzaldehyde, according to the general procedure the *title compound* was obtained as a white solid (1.38g, 83%) m.p. 166.0-166.8ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.44 (s, 3H, CH_3), 3.97 (s, 3H, OMe), 4.75 (br s, 1H, OH), 7.07 (br s, 1H, ArH), 7.34 (d, *J*=8.8Hz, 2H, ArH), 7.70 (br s, 1H, ArH), 7.89 (d, *J*=8.8Hz, 2H, ArH), 9.29 (br s, 1H, HC=N) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.8 (CH_3), 56.7 (OMe), 115.4 (CH), 121.0 (C), 124.6 (C), 126.6 (CH), 128.3 (2xCH), 129.9 (2xCH), 135.4 (C), 144.7 (C), 145.5 (C), 152.7 (C), 168.7 (HC=N) ppm.

5H-Dibenzo[b,e][1,4]diazepine (4aa) *was prepared by two other pathways:*

According to Scheme 4, pathway b in the main text.

o-Bromobenzaldehyde (0.200g, 1.08 mmol), $Pd(OAc)_2$ (2.5mol%), SPhos (5.0 mol%), 4-methylbenzenesulfonamide (1 equiv), Cs_2CO_3 (2 equivs) and THF were added to a reaction tube and heated at 100ºC for 2h. The reaction mixture was allowed to cool and then *o*-bromoaniline (1 equiv) was added and the reaction was heated at 100ºC for 18 h. The reaction mixture was cooled to room temperature. The reaction mixture was filtered through celite and the solvent removed by evaporation under reduced pressure and, after purification by silica gel column chromatography using 9:1 hexane / EtOAc as the eluent, the *title compound* was obtained as a yellow solid (0.081 g, 39%).

According to Scheme 5 in the main text.

2-(2-Bromophenylamino)benzaldehyde (0.254g, 0.92mol), $Pd(OAc)_2$ (2.5mol%), SPhos (5.0 mol%), 4-methylbenzenesulfonamide (1 equiv), Cs_2CO_3 (2 equivs) and THF were heated in a tube 100ºC for 18h. The reaction mixture was allowed to cool to room temperature and then filtered through celite and the solvent was removed by evaporation under reduced pressure and, after purification by silica gel column chromatography using 9: 1 hexane / EtOAc as the eluent, the *title compound* was obtained as a yellow solid (0.018 g, 10%).

NMR Spectra (^{1}H 400MHz; ^{13}C 100MHz) of the aldimine substrates (2):

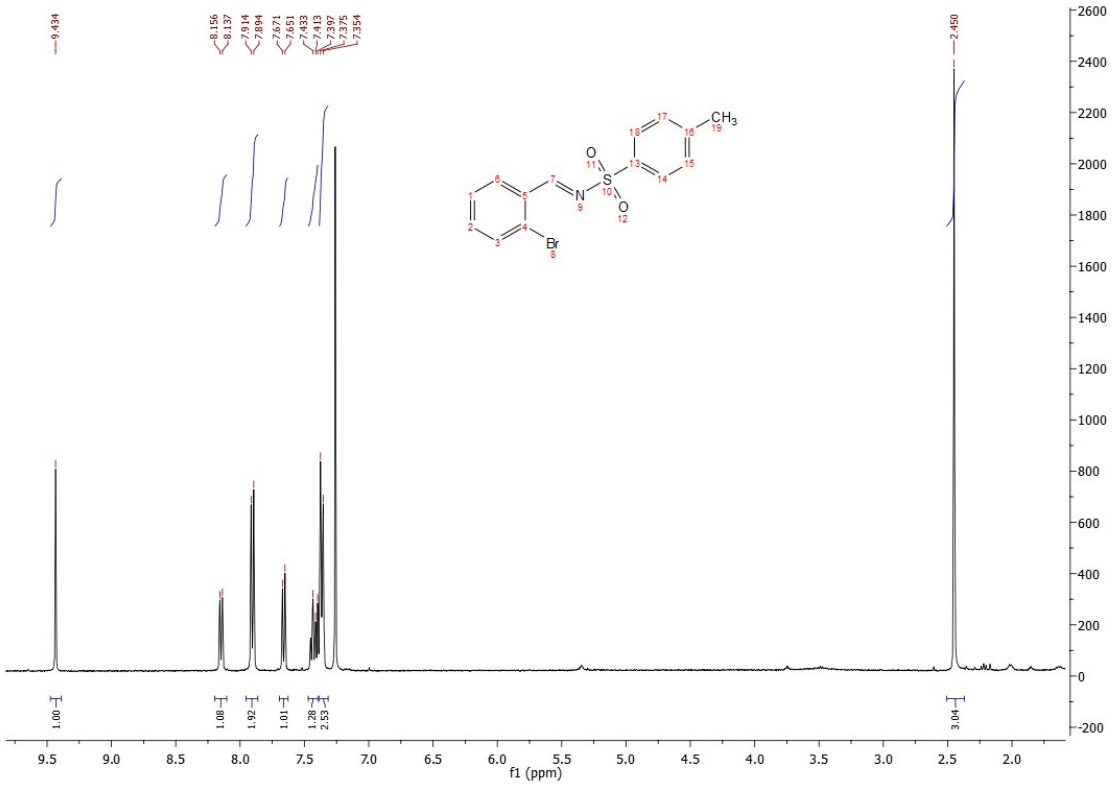


Figura S1. ^{1}H NMR spectrum of *N*-(2-bromobenzylidene)-4-methylbenzenesulfonamide (**2a**) in $CDCl_3$.

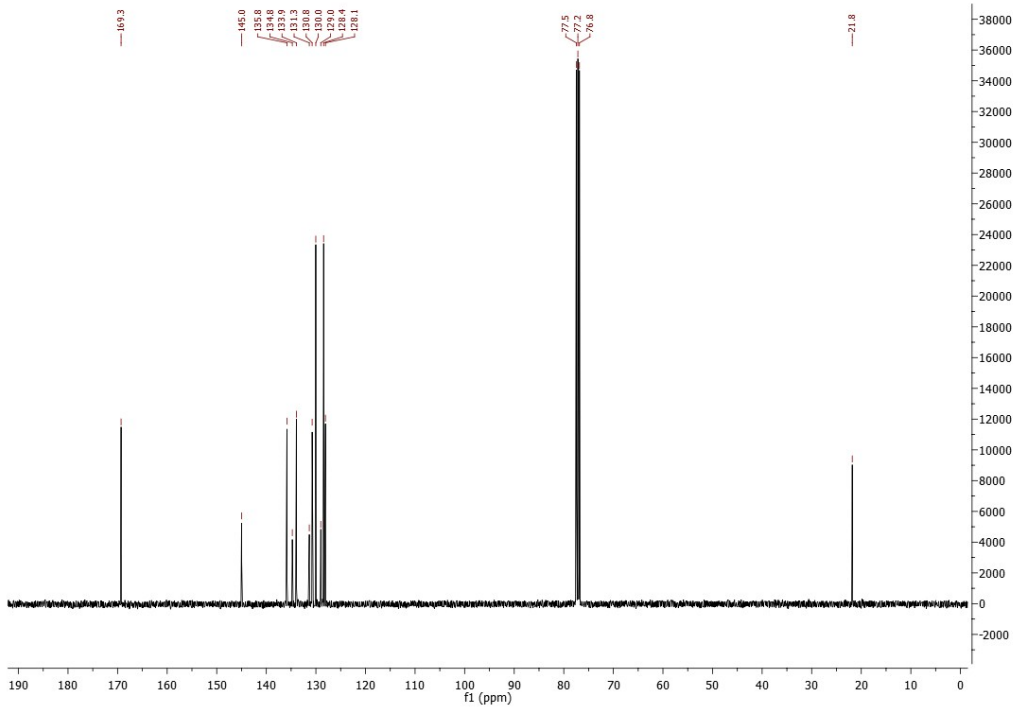


Figura S2. ^{13}C NMR spectrum of *N*-(2-bromobenzylidene)-4-methylbenzenesulfonamide (**2a**) in $CDCl_3$**.**

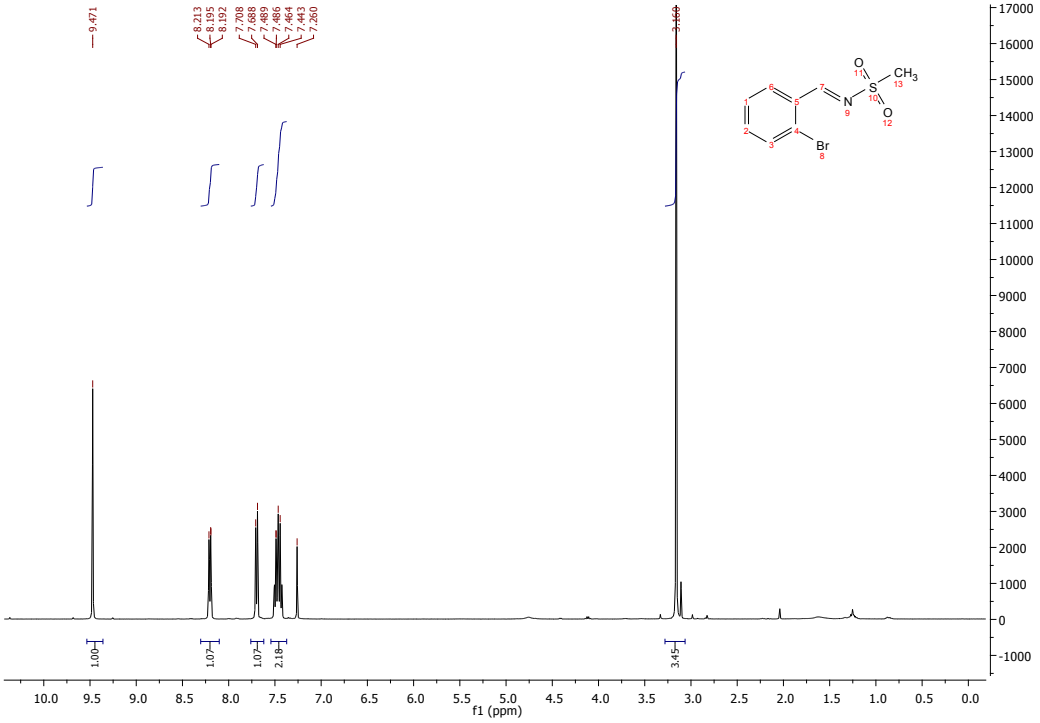


Figure S3. ^{1}H NMR spectrum of *N*-(2-Bromobenzylidene)methanesulfonamide (**2b**) in $CDCl_3$.

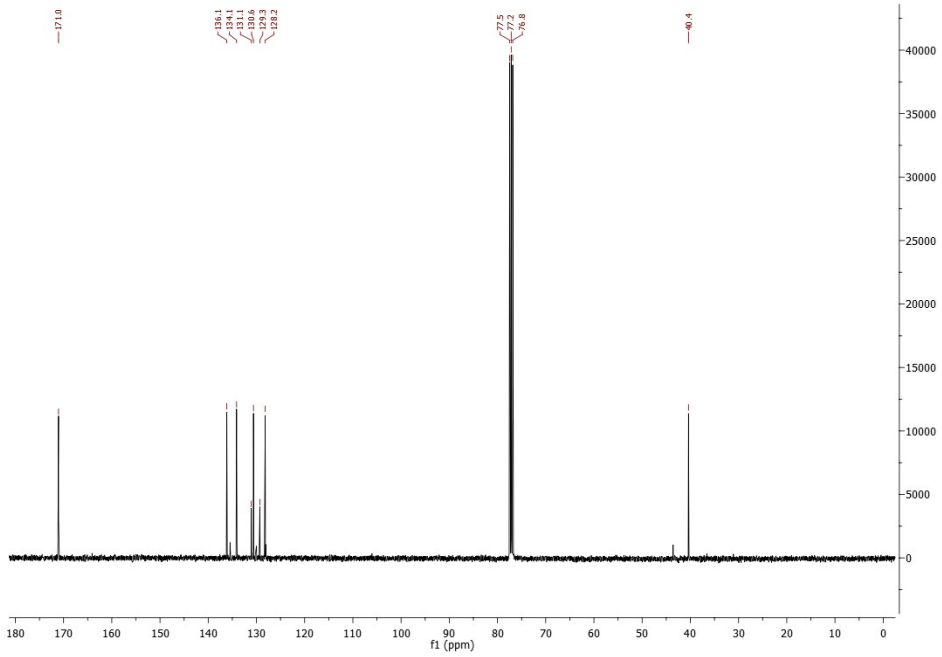


Figure S4. ^{13}C NMR spectrum of *N*-(2-Bromobenzylidene)methanesulfonamide (**2b**) in $CDCl_3$.

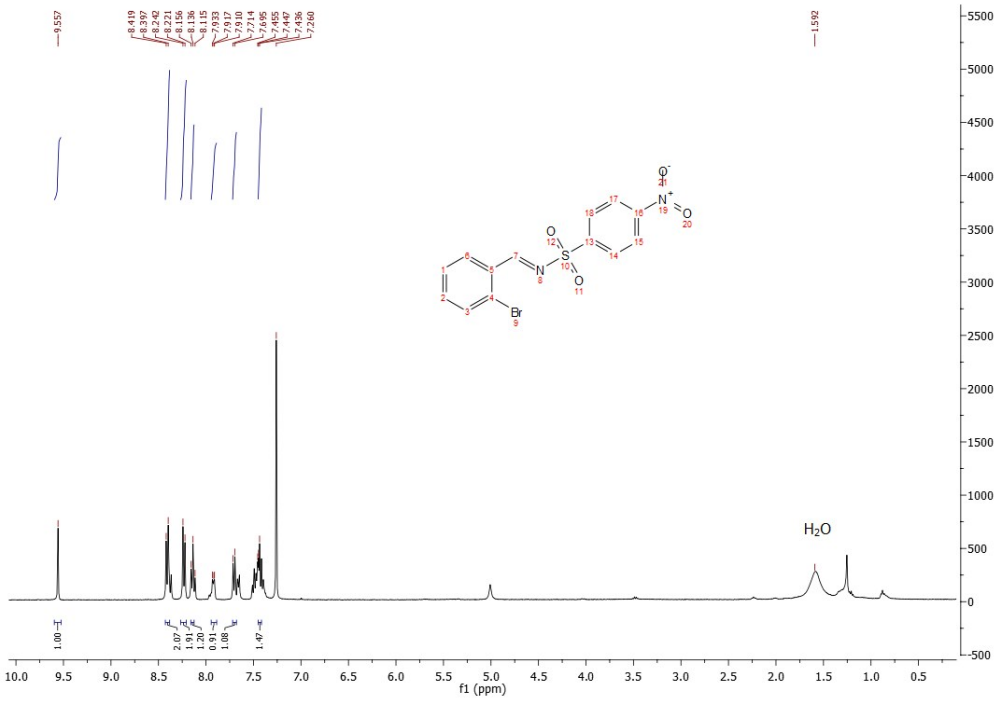


Figure S5. ^{1}H NMR spectrum of *N*-(2-Bromobenzylidene)-4-nitrobenzenesulfonamide (**2c**) in $CDCl_3$.

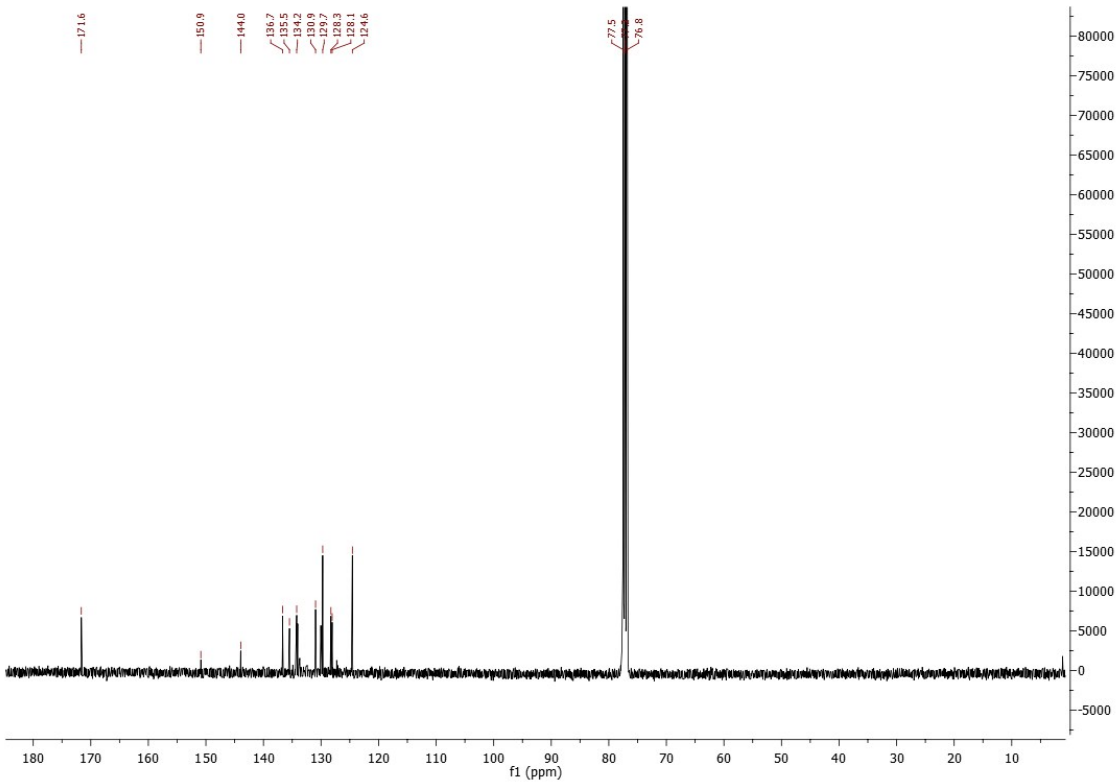


Figure S6. ^{13}C NMR spectrum of *N*-(2-Bromobenzylidene)-4-nitrobenzenesulfonamide (**2c**) in $CDCl_3$.

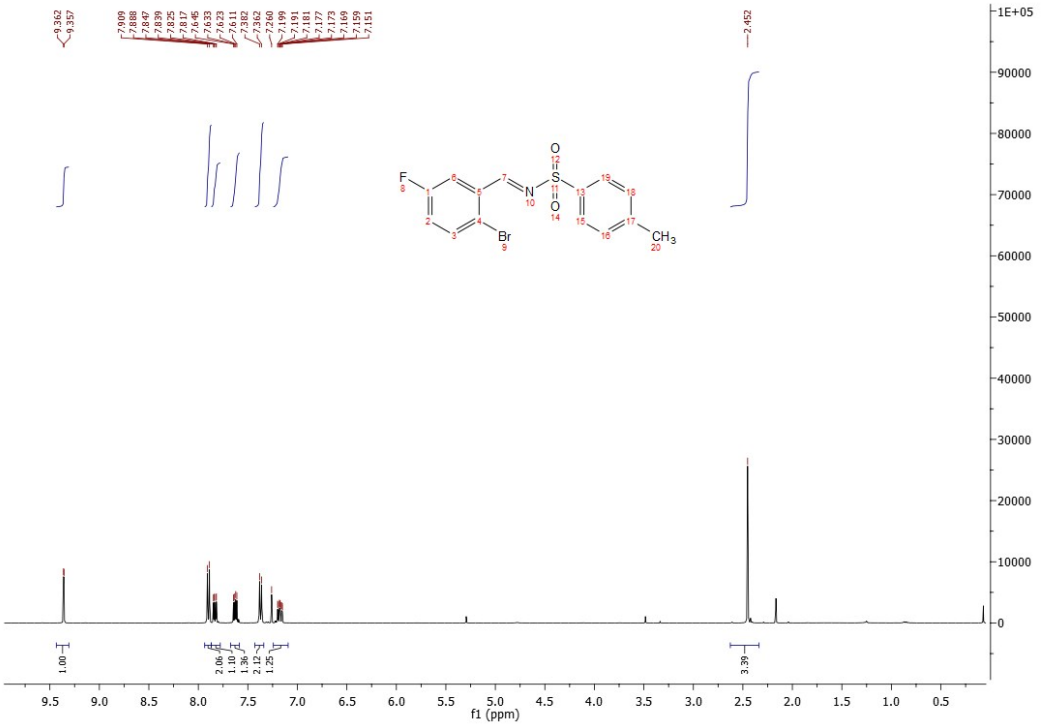


Figure S7. ^{1}H NMR spectrum of *N*-(2-bromo-5-fluorobenzylidene)-4-methylbenzenesulfonamide (**2d**) in $CDCl_3$

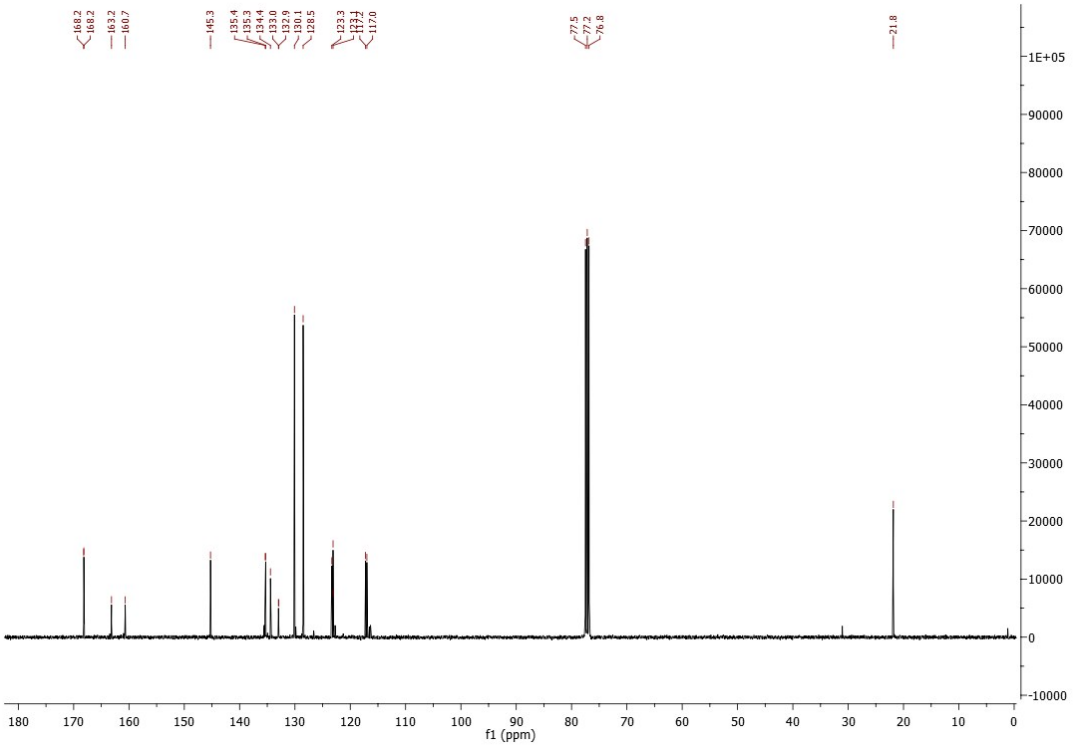


Figure S8. ^{13}C NMR spectrum of of *N*-(2-bromo-5-fluorobenzylidene)-4-methylbenzenesulfonamide (**2d**) in $CDCl_3$.

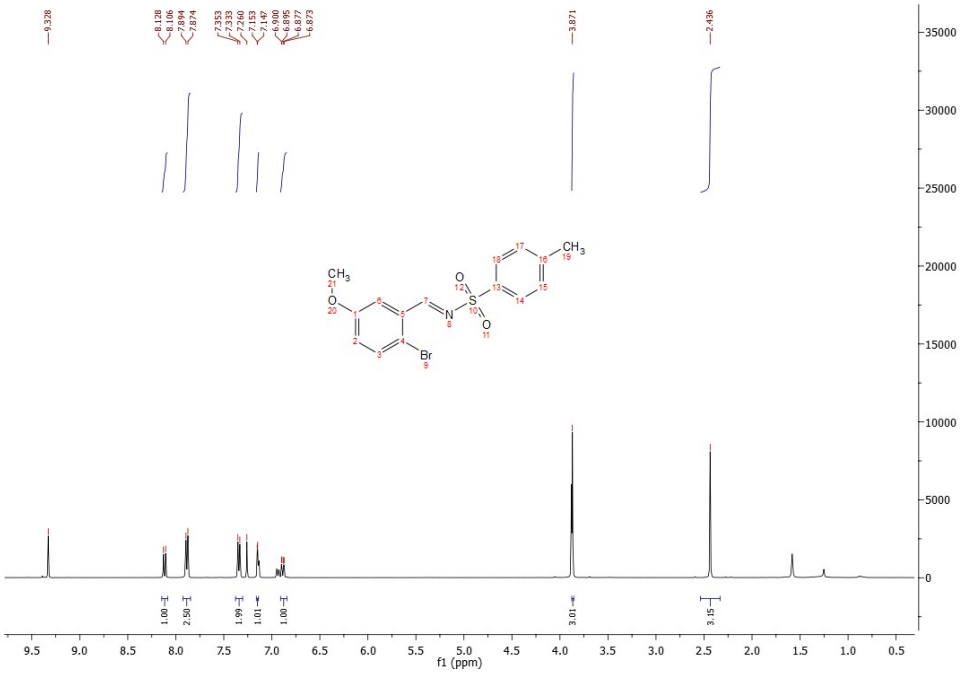


Figure S9. ^{1}H NMR spectrum of *N*-(2-Bromo-4-methoxybenzylidene)-4-methylbenzenesulfonamide (**2f**) in $CDCl_3$.

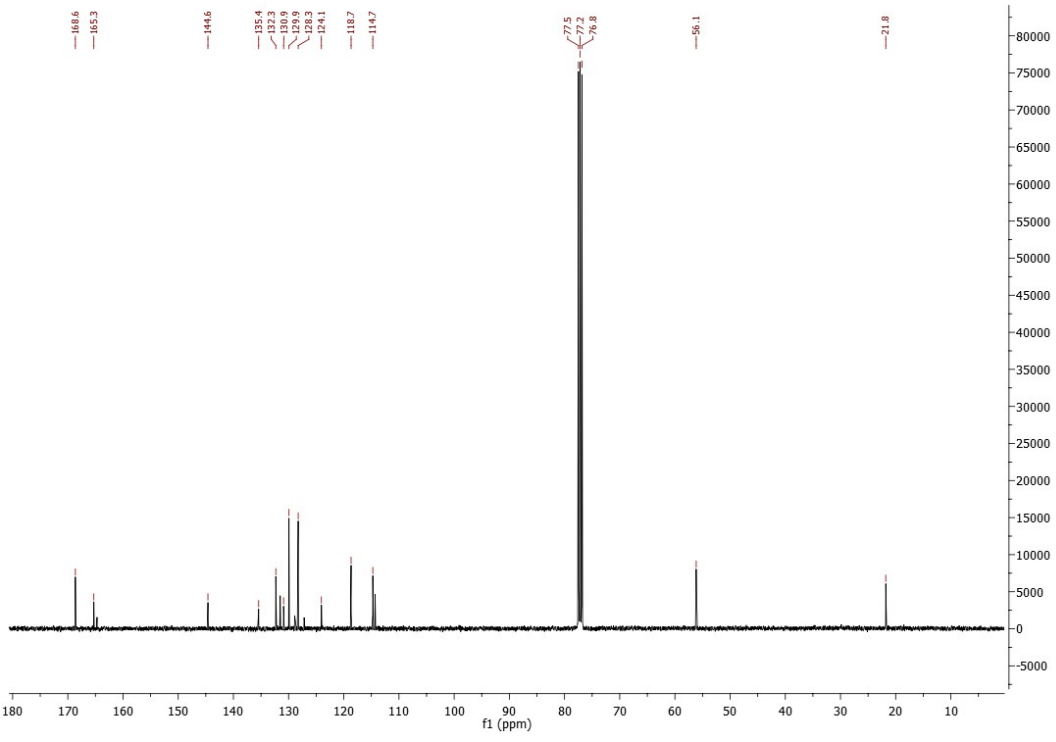


Figure S10. ^{13}C NMR spectrum of *N*-(2-Bromo-4-methoxybenzylidene)-4-methylbenzenesulfonamide (**2f**) in $CDCl_3$.

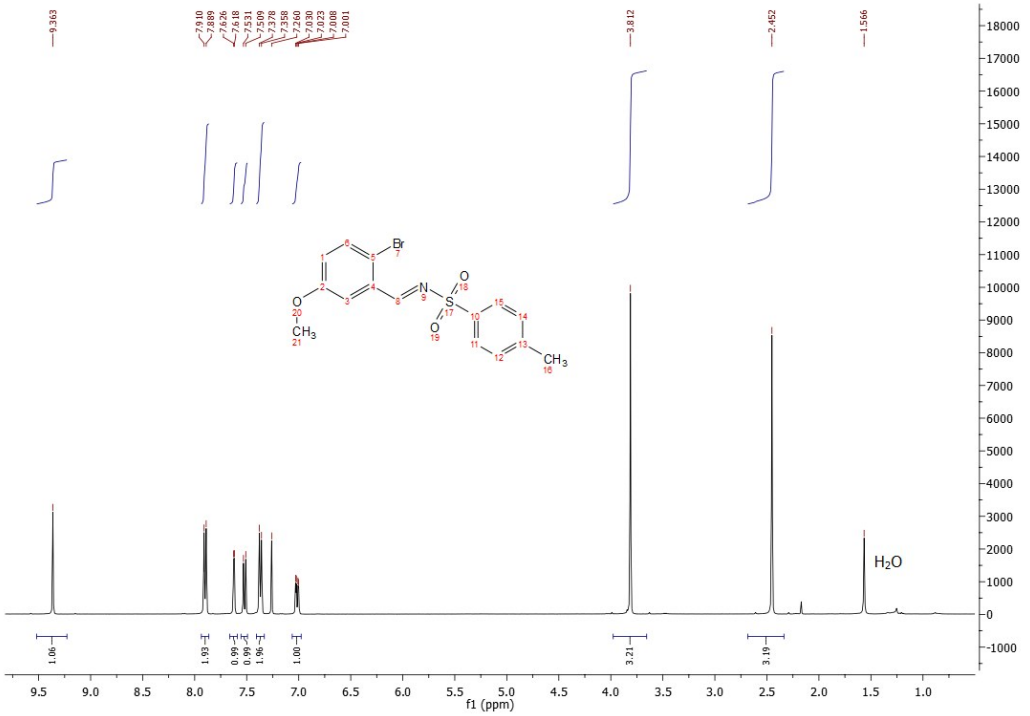


Figure S11. ^{1}H NMR spectrum of *N*-(2-Bromo-5-methoxybenzylidene)-4-methylbenzenesulfonamide (**2e**) in $CDCl_3$.

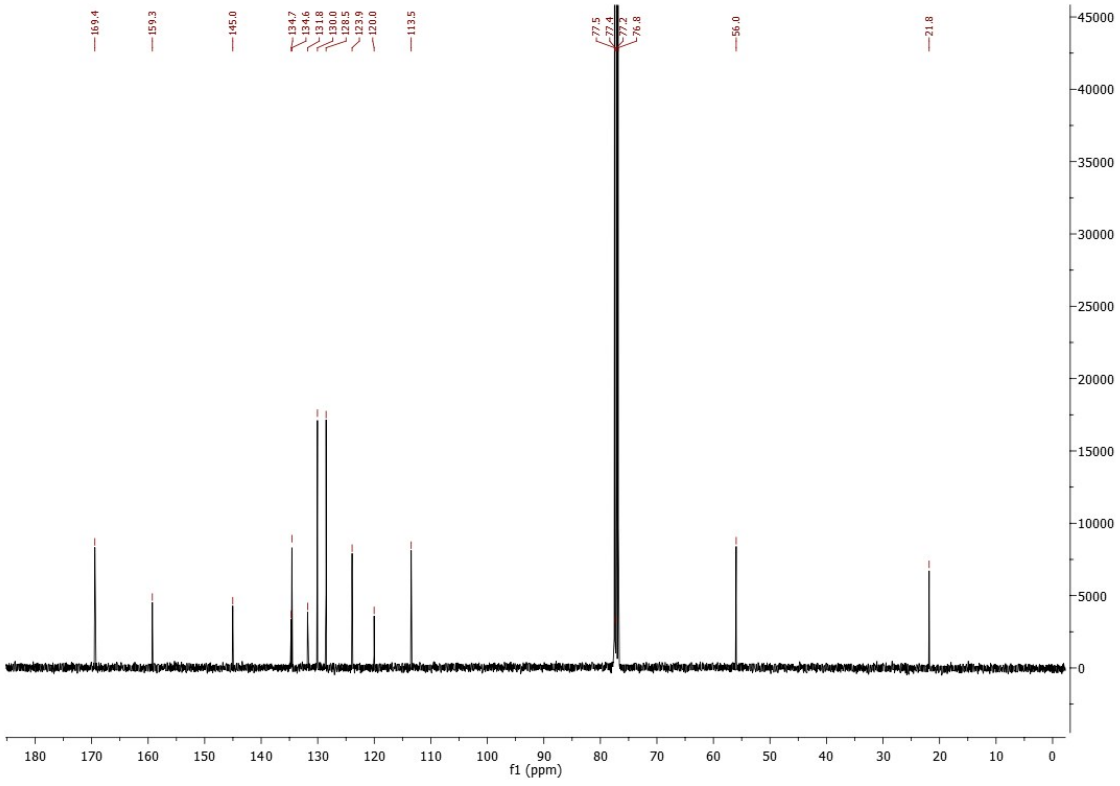


Figure S12. ^{13}C NMR spectrum of *N*-(2-Bromo-5-methoxybenzylidene)-4-methylbenzenesulfonamide (**2e**) in $CDCl_3$.

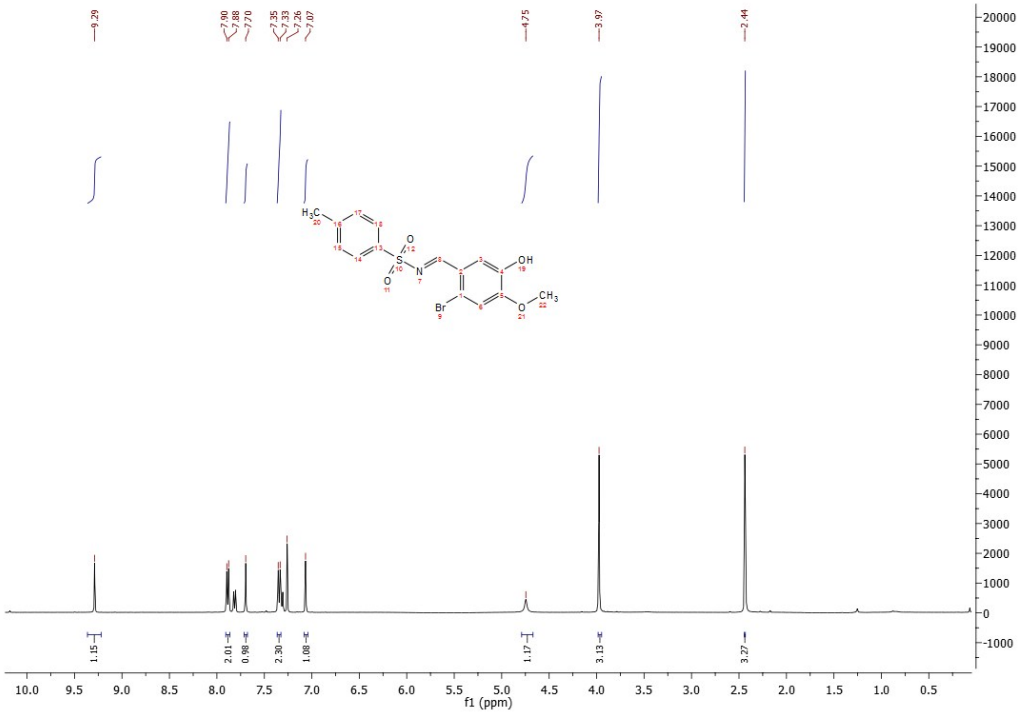


Figure S13. ^{1}H NMR spectrum of *N*-(2-Bromo-5-hydroxy-4-methoxybenzylidene)-4-methylbenzenesulfonamide (**2g**) in $CDCl_3$.

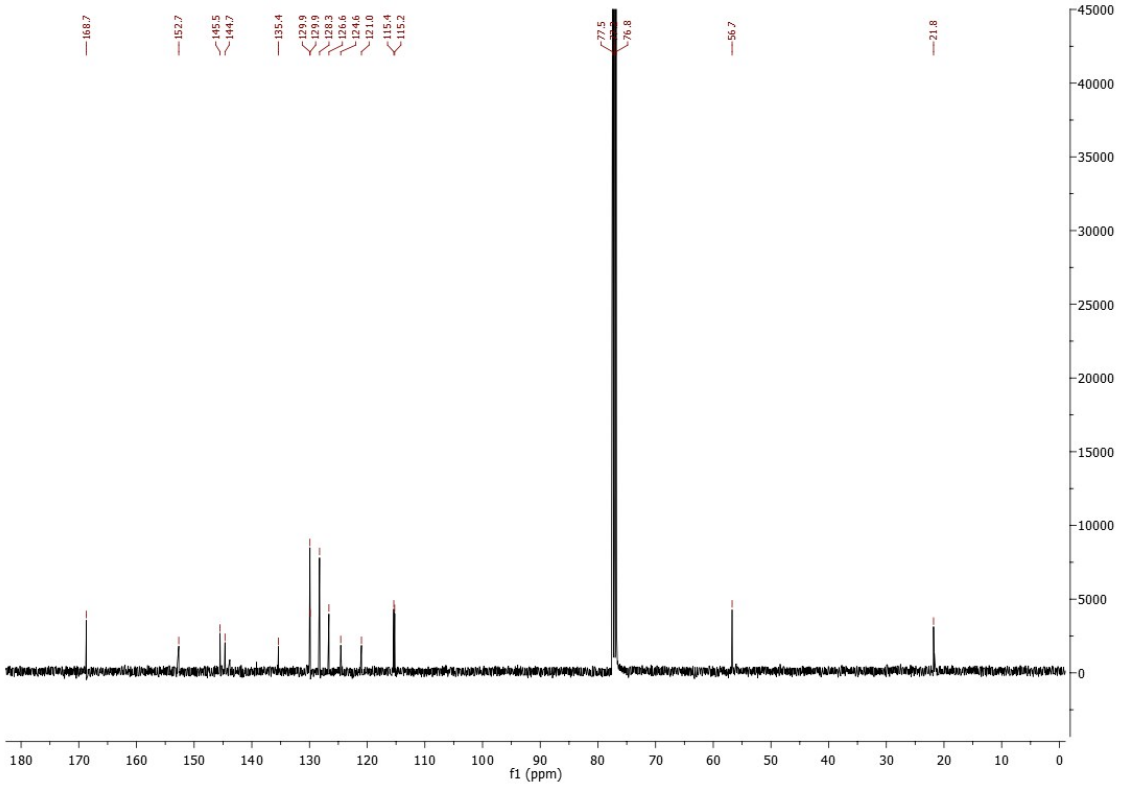


Figure S14. ^{13}C NMR spectrum of *N*-(2-Bromo-5-hydroxy-4-methoxybenzylidene)-4-methylbenzenesulfonamide (**2g**) in $CDCl_3$.

NMR Spectra (^{1}H 400MHz; ^{13}C 100MHz) for DBDA (4) and compounds (5) and (6):

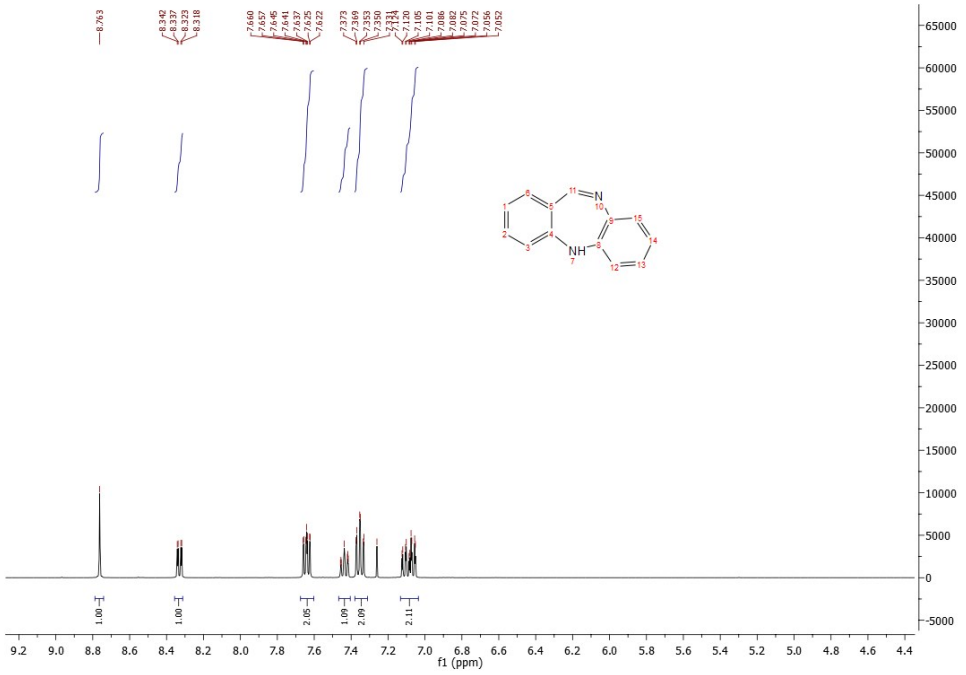


Figure S15. ^{1}H NMR spectrum of 5*H*-dibenzo[*b*,*e*][1,4]diazepine **(4aa)** in $CDCl_3$.

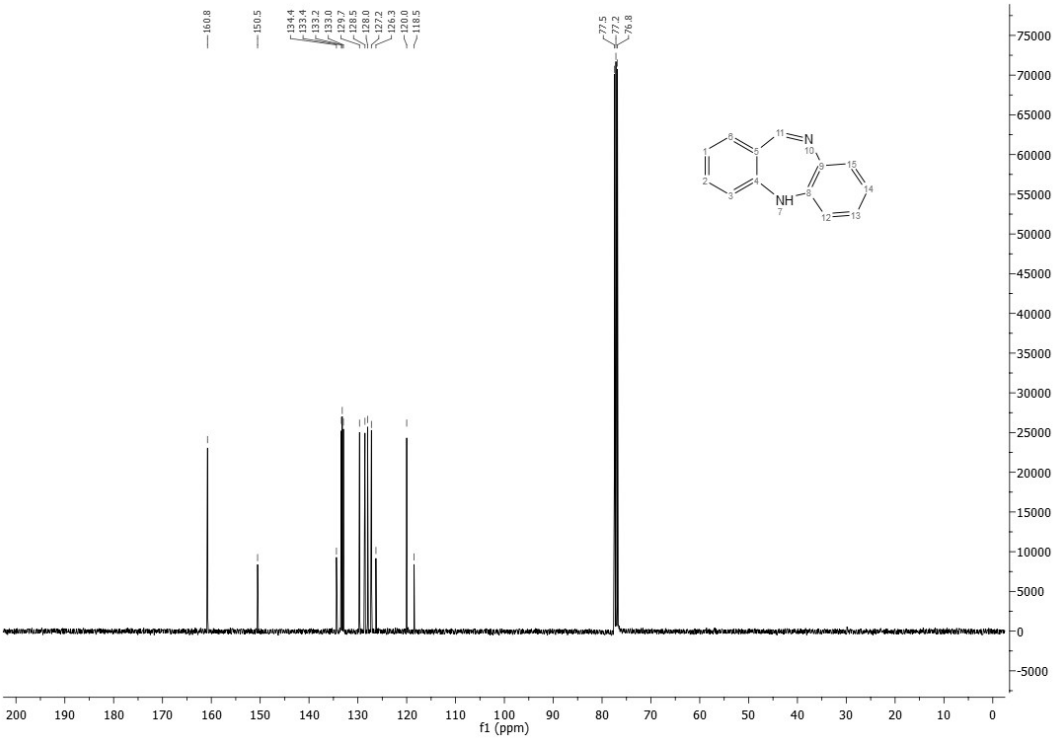


Figure S16. ^{13}C NMR spectrum of 5*H*-dibenzo[*b*,*e*][1,4]diazepine **(4aa)** in $CDCl_3$.

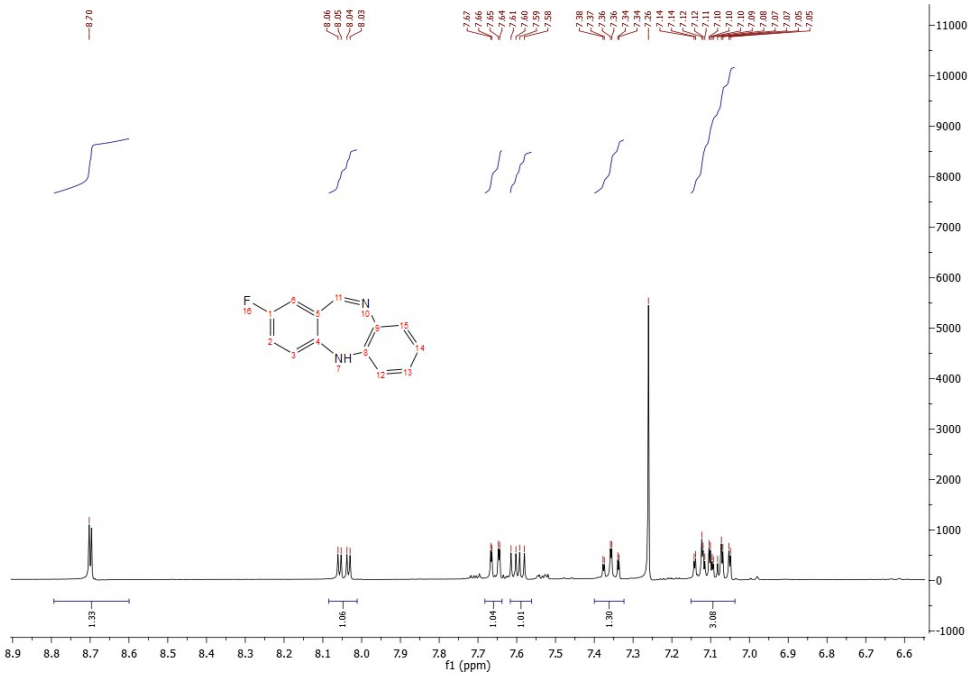


Figure S17. ^{1}H NMR spectrum of 2-fluoro-5*H*-dibenzo[*b*,*e*][1,4]diazepine (**4da**) in $CDCl_3$.

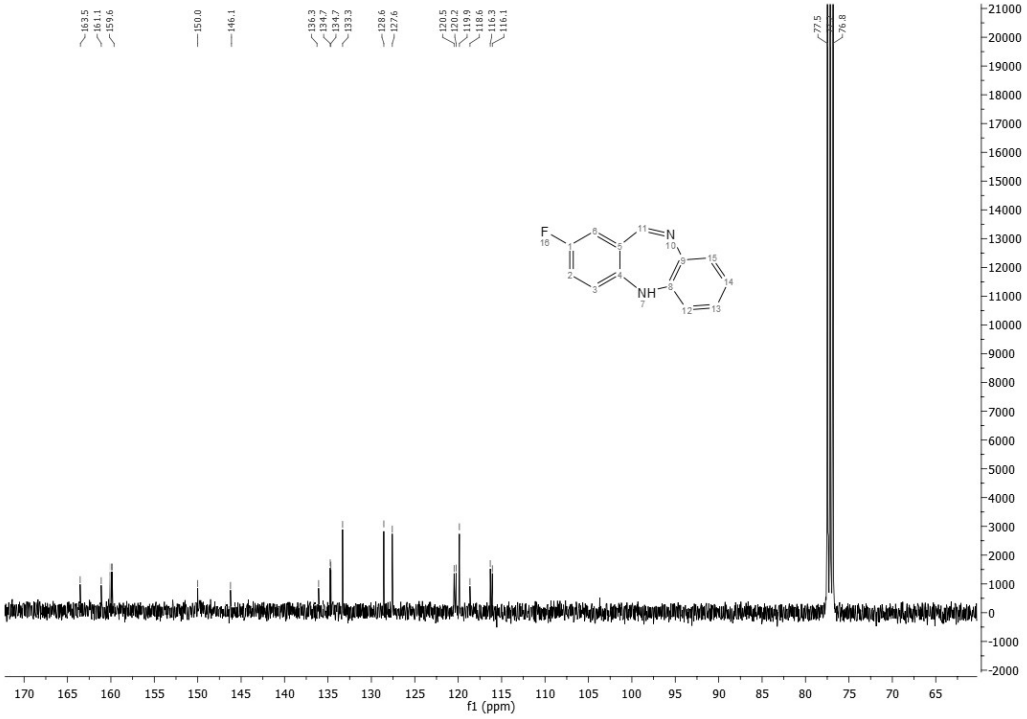


Figure S18. ^{13}C NMR spectrum of 2-fluoro-5*H*-dibenzo[*b*,*e*][1,4]diazepine (**4da**) in $CDCl_3$.

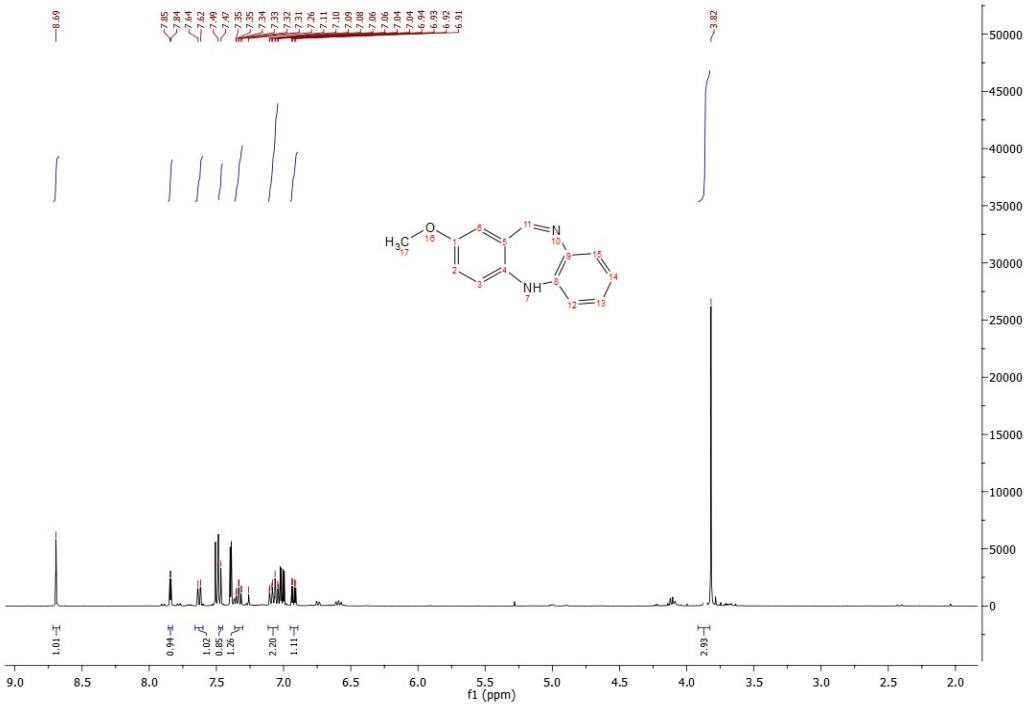


Figure S19. ^{1}H NMR spectrum of 2-methoxy-5*H*-dibenzo[*b*,*e*][1,4]diazepine (**4ea**) in $CDCl_3$.

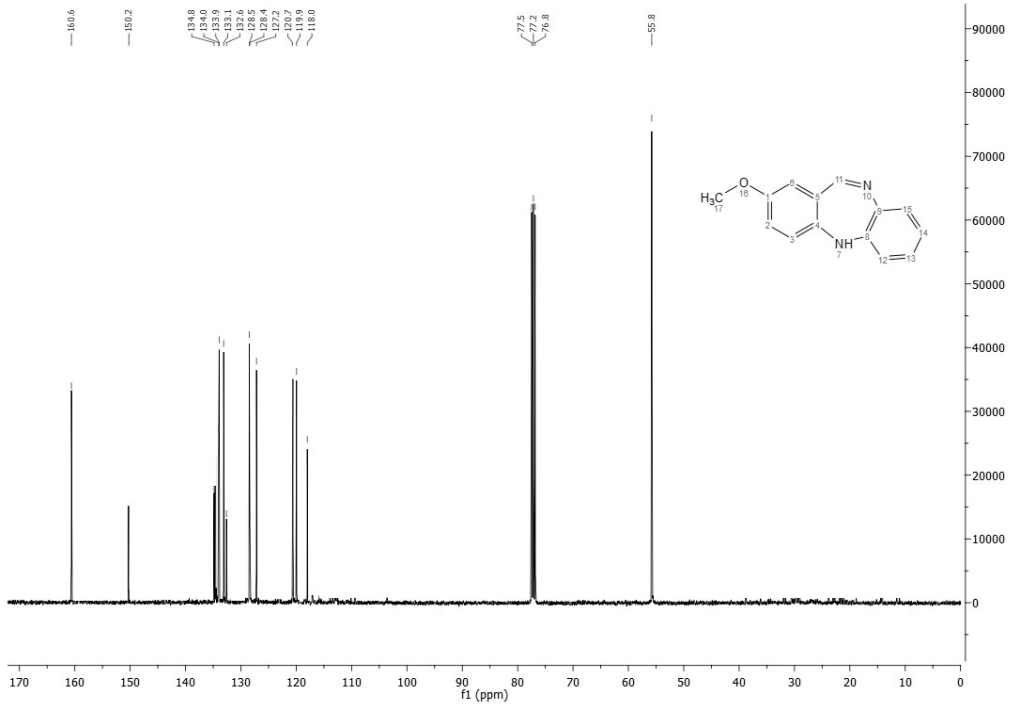


Figure S20. ^{13}C NMR spectrum of 2-methoxy-5*H*-dibenzo[*b*,*e*][1,4]diazepine (**4ea**) in $CDCl_3$.

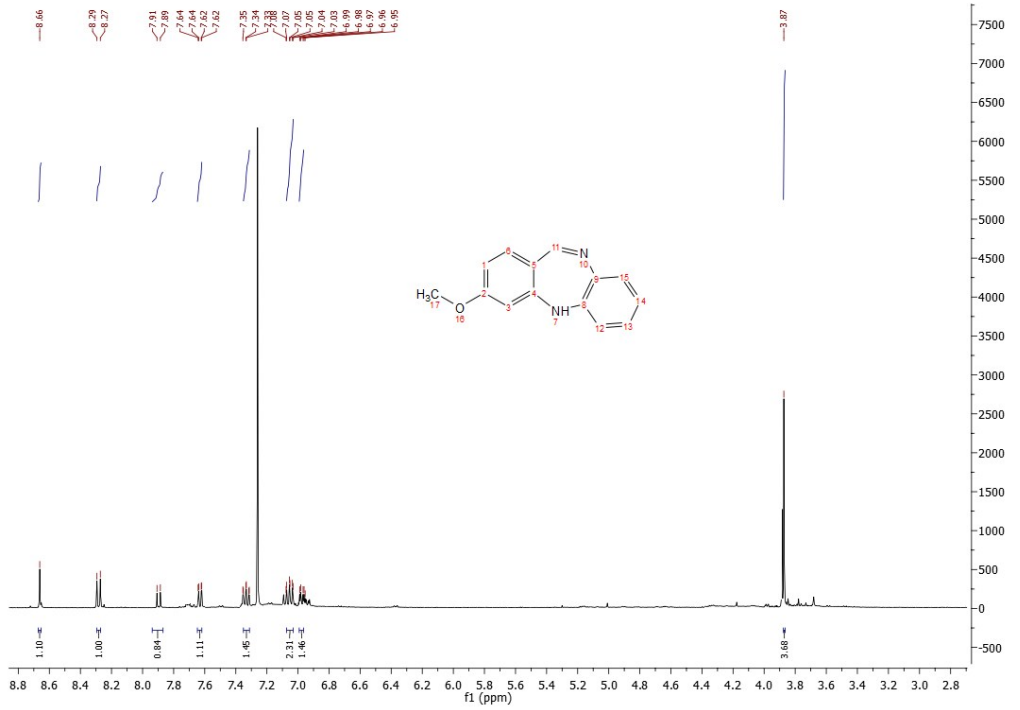


Figure S21. ^{1}H NMR spectrum of 3-methoxy-5*H*-dibenzo[*b*,*e*][1,4]diazepine (**4fa**) in $CDCl_3$.

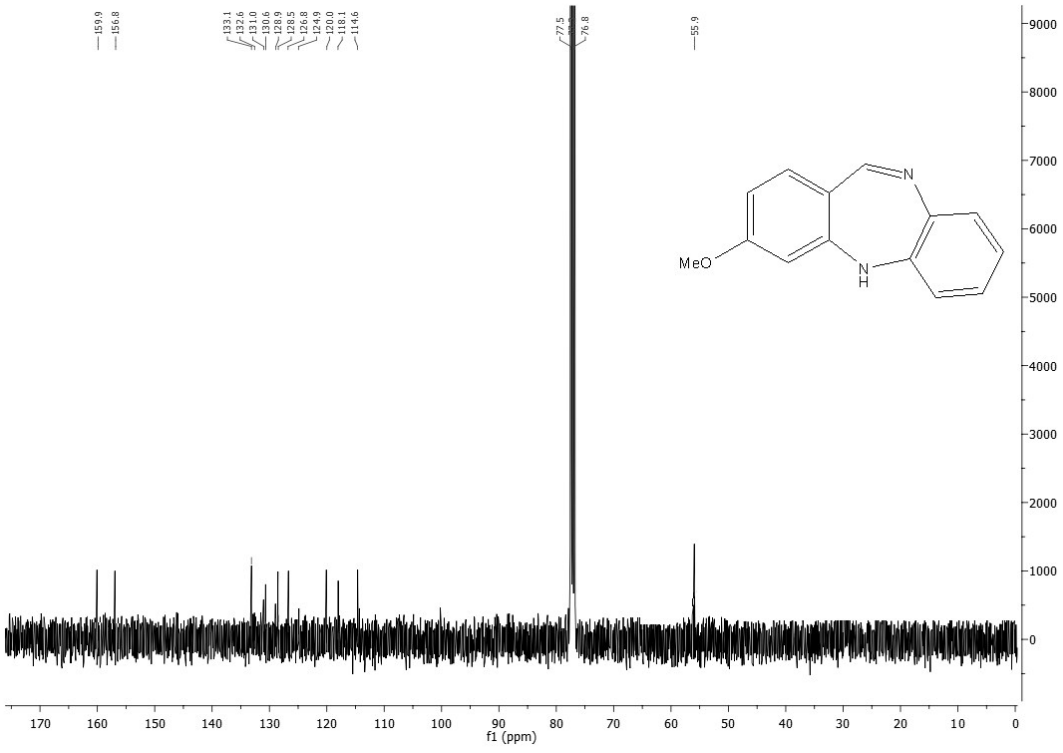


Figure S22. ^{13}C NMR spectrum of 3-methoxy-5*H*-dibenzo[*b*,*e*][1,4]diazepine (**4fa**) in $CDCl_3$.

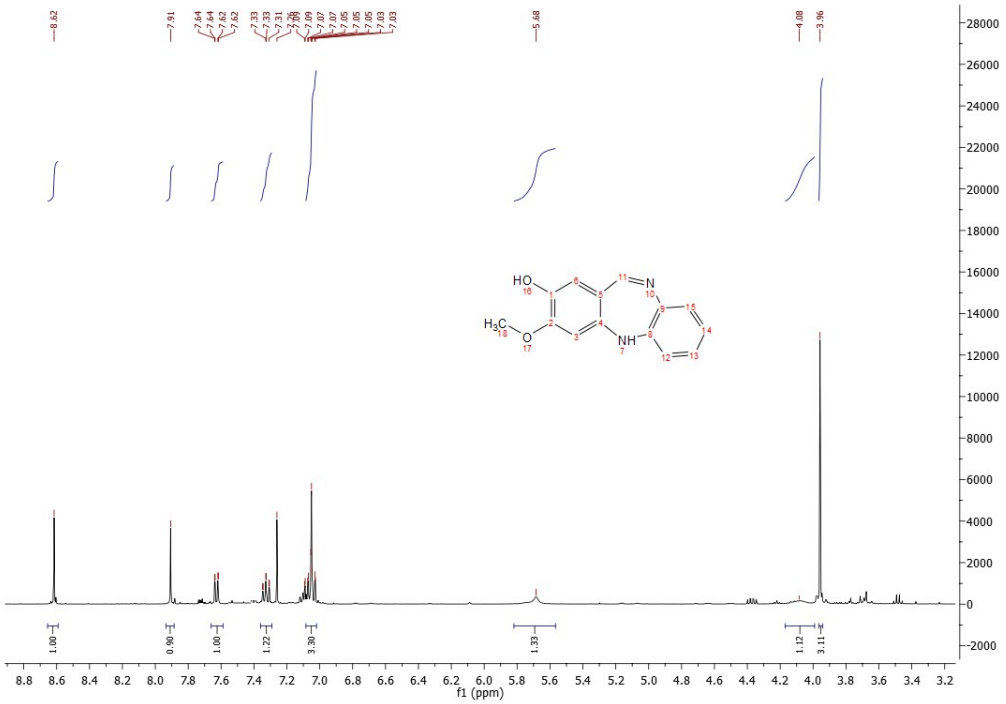


Figure S23. ^{1}H NMR spectrum of 3-methoxy-5*H*-dibenzo[*b*,*e*][1,4]diazepin-2-ol (**4ga**) $CDCl_3$.

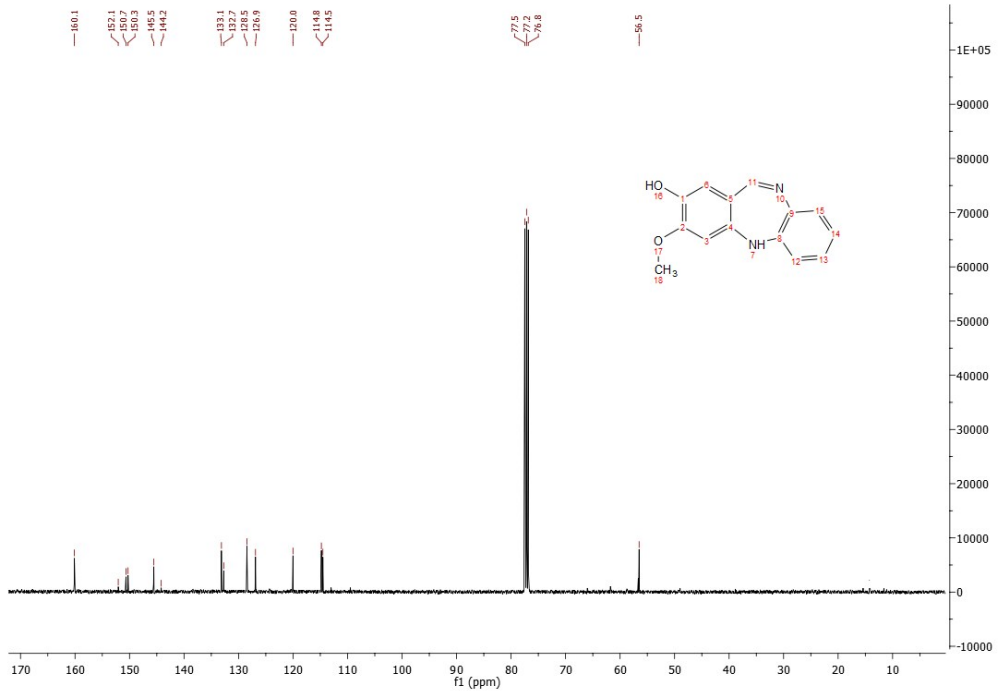


Figure S24. ^{13}C NMR spectrum of 3-methoxy-5*H*-dibenzo[*b*,*e*][1,4]diazepin-2-ol (**4ga**) in $CDCl_3$.

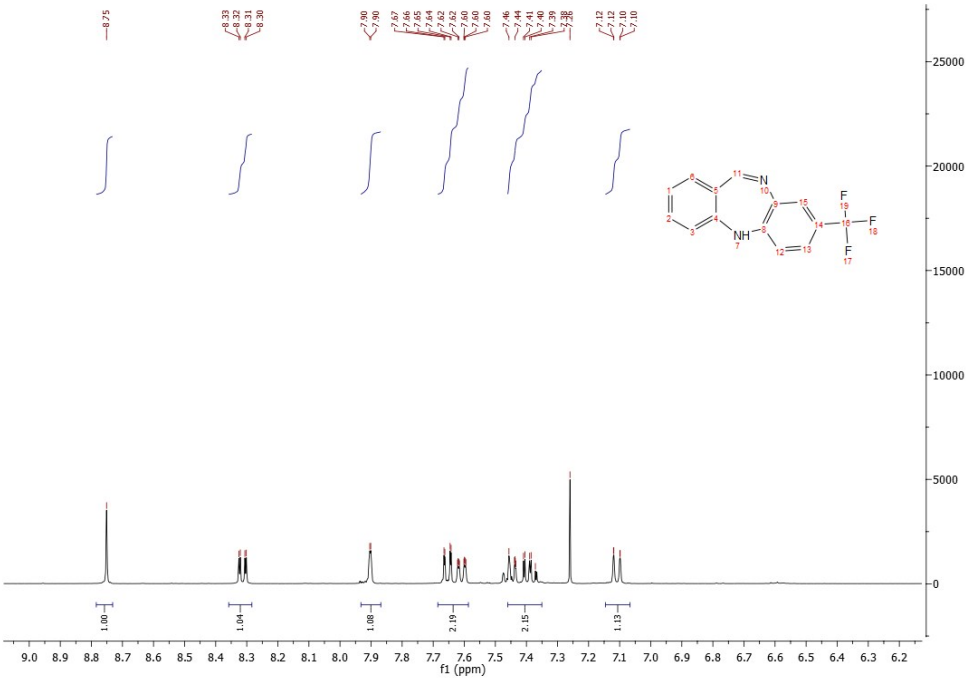


Figure S25. ^{1}H NMR spectrum of 8-(trifluoromethyl)-5*H*-dibenzo[*b*,*e*][1,4]diazepine (**4ab**) in $CDCl_3$.

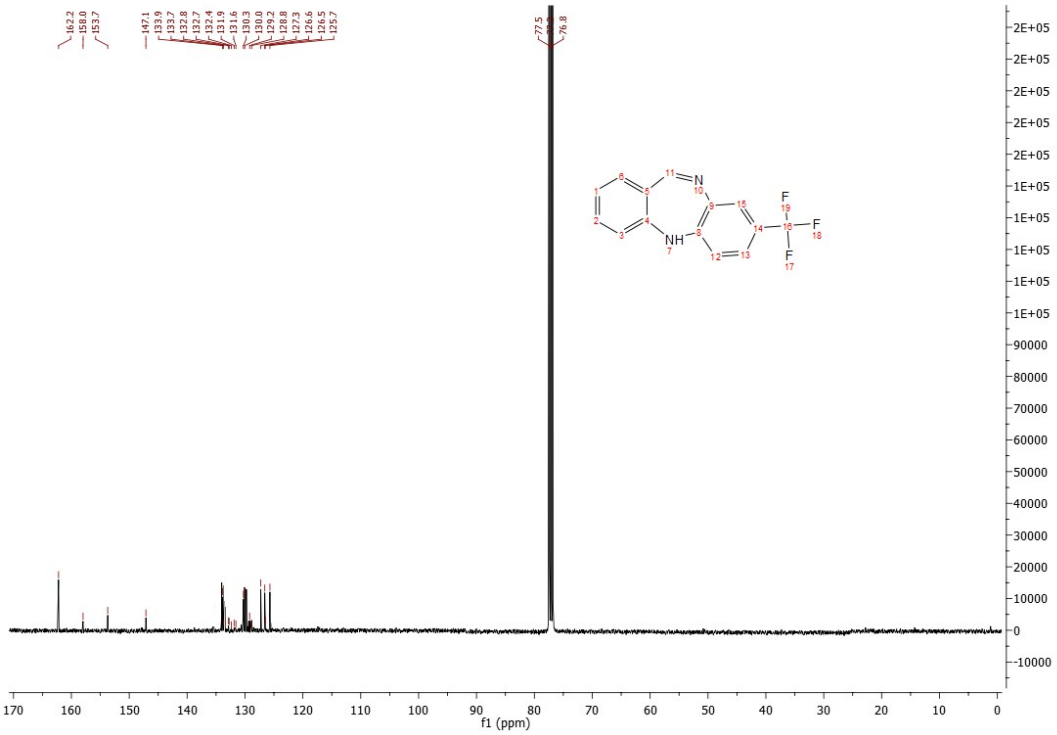


Figure S26. ^{13}C NMR spectrum of 8-(trifluoromethyl)-5*H*-dibenzo[*b*,*e*][1,4]diazepine (**4ab**) in $CDCl_3$.

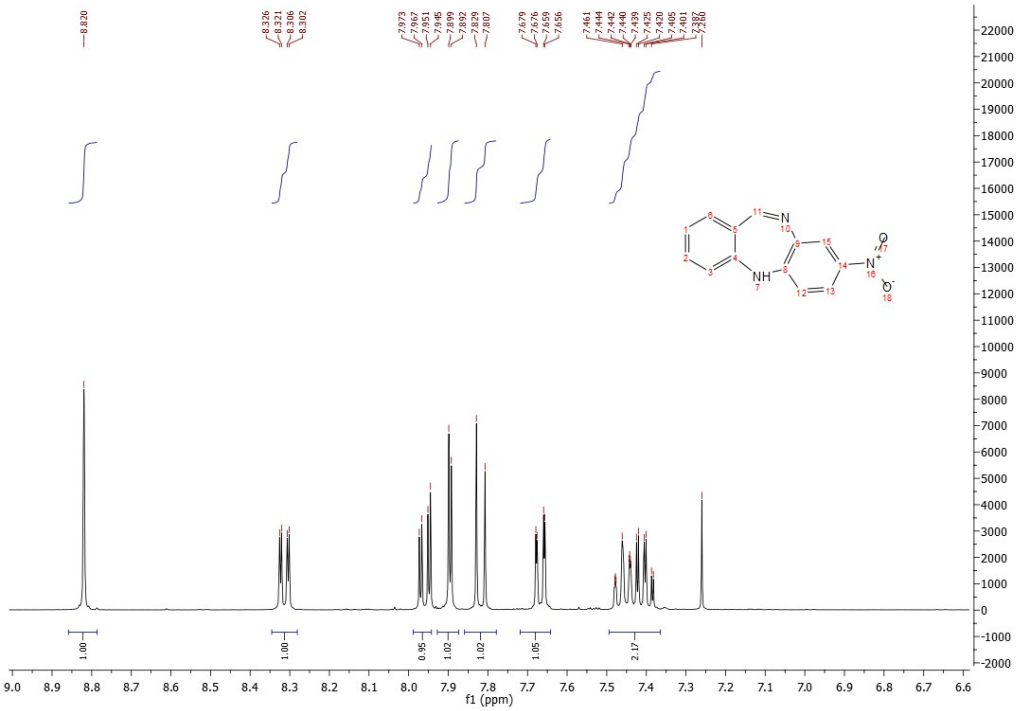


Figure S27. ^{1}H NMR spectrum of 7-nitro-5*H*-dibenzo[*b*,*e*][1,4]diazepine (**4ad**) in $CDCl_3$.

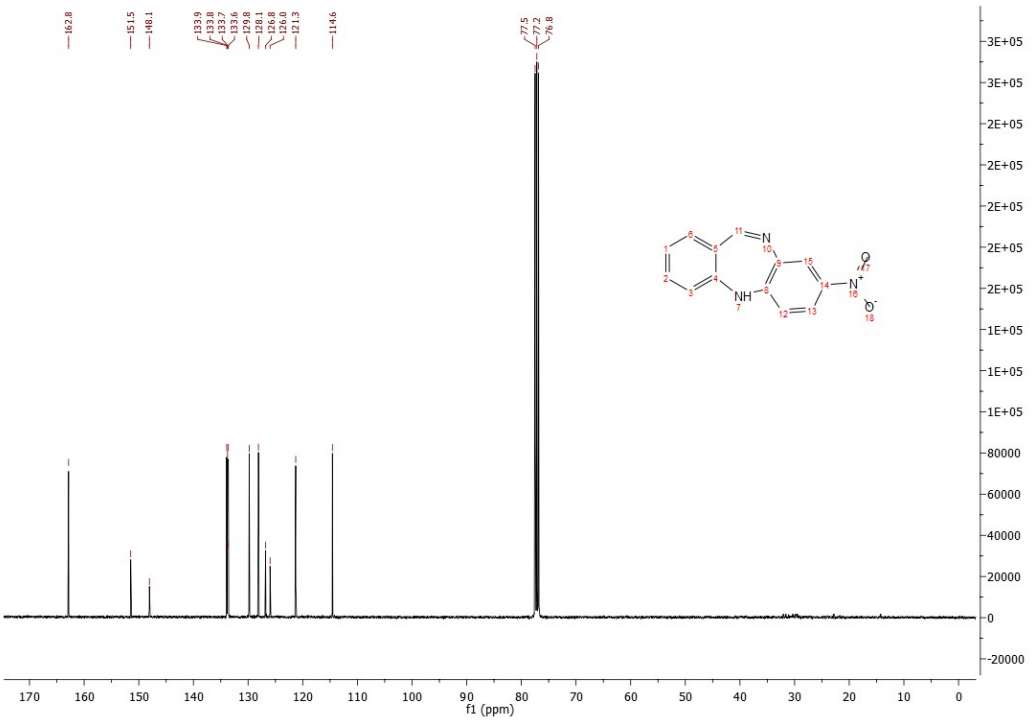


Figure S28. ^{13}C NMR spectrum of 7-nitro-5*H*-dibenzo[*b*,*e*][1,4]diazepine (**4ad**) in $CDCl_3$.

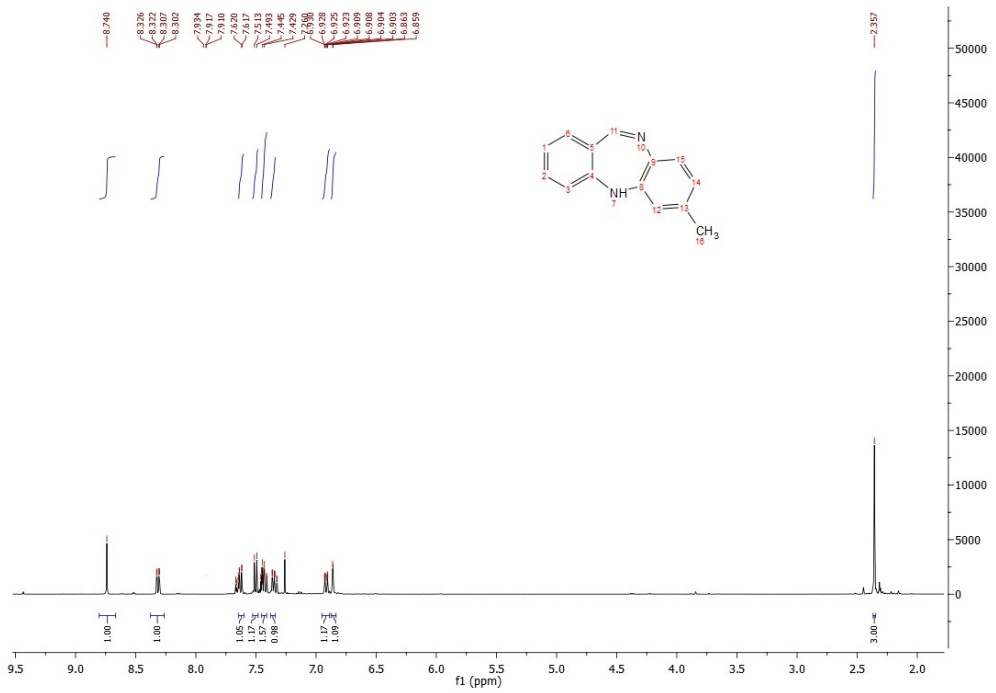


Figure S29. ^{1}H NMR spectrum of 7-methyl-5H-dibenzo[*b*,*e*][1,4]diazepine (**4ac**) in $CDCl_3$.

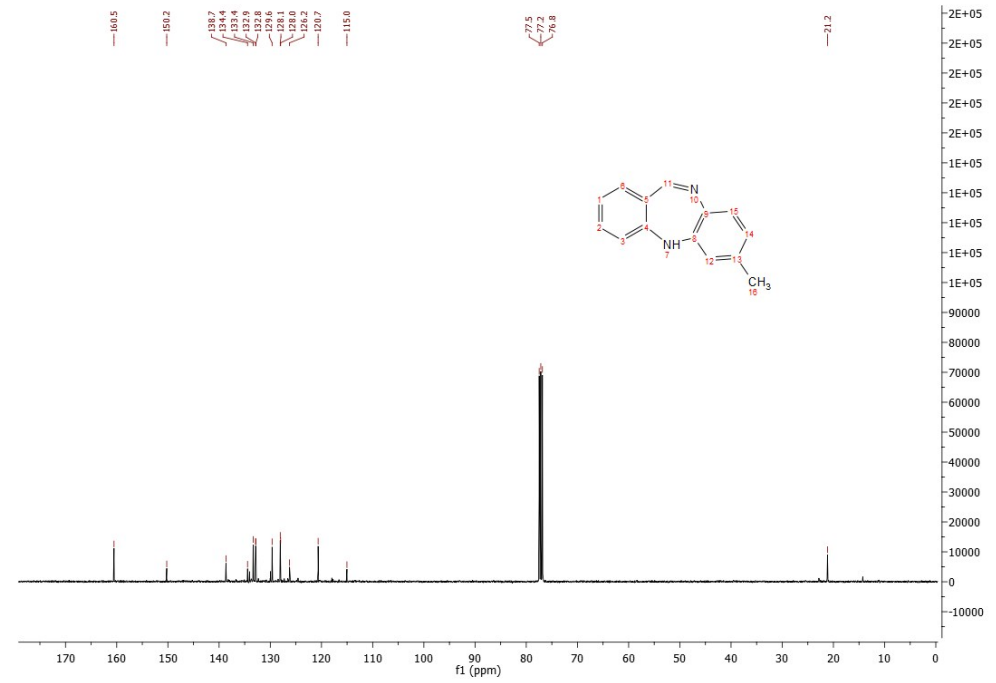


Figure S30. ^{13}C NMR spectrum of 7-methyl-5H-dibenzo[*b*,*e*][1,4]diazepine (**4ac**) in $CDCl_3$.

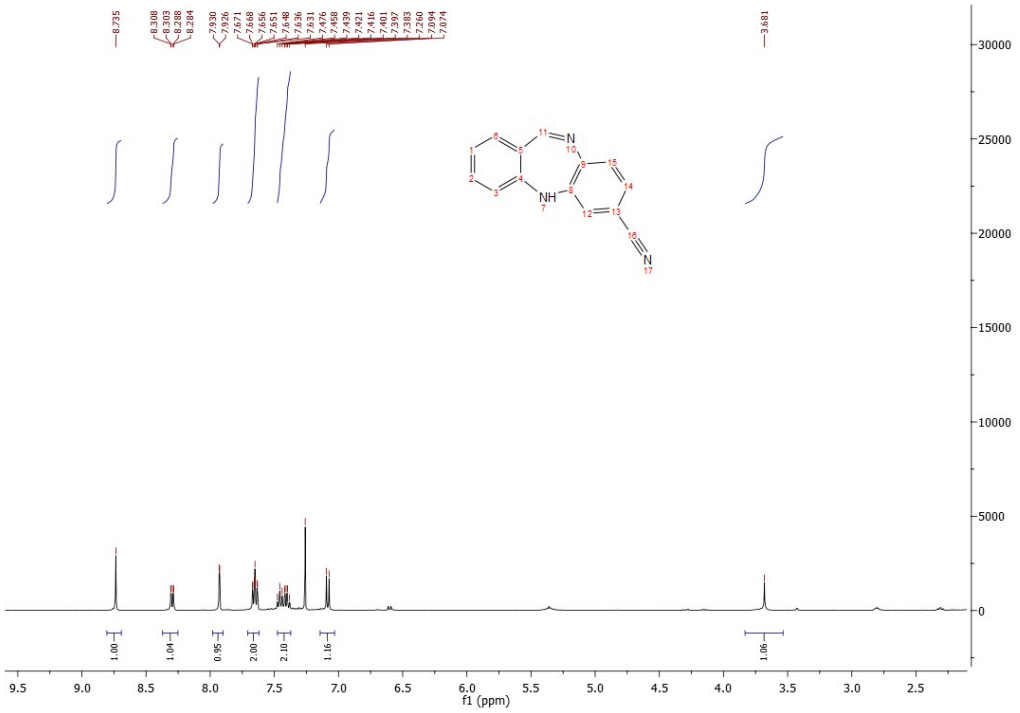


Figure S31. ^{1}H NMR spectrum of 5*H*-dibenzo[b,e][1,4]diazepine-7-carbonitrile (**4ae**) in $CDCl_3$.

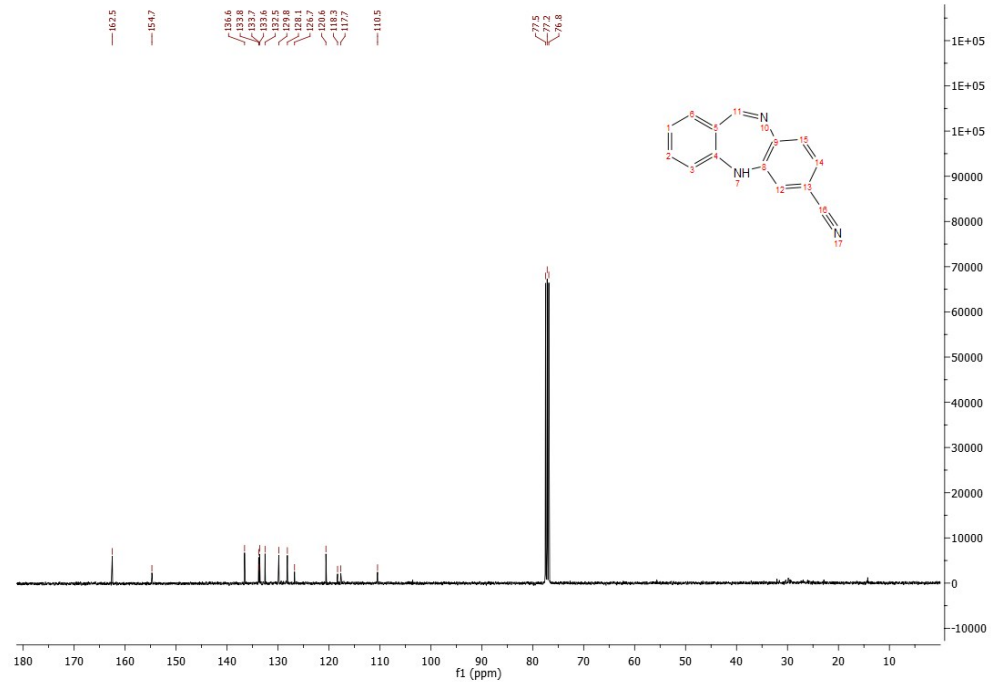


Figure S32. ^{13}C NMR spectrum of 5*H*-dibenzo[b,e][1,4]diazepine-7-carbonitrile (**4ae**) in $CDCl_3$.

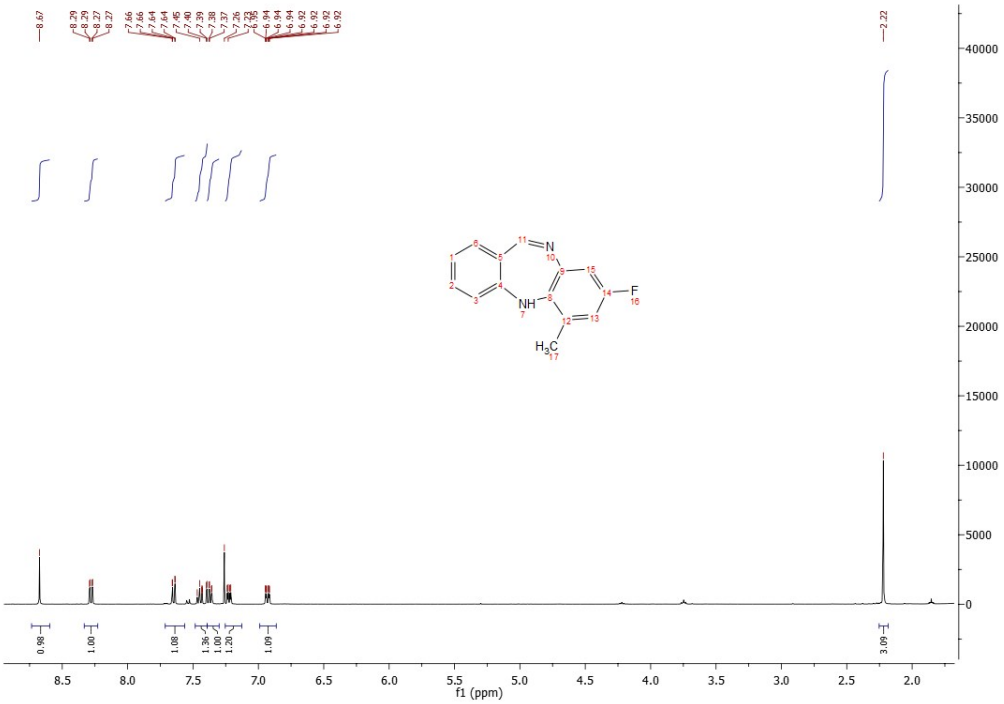


Figure S33. ^{1}H NMR spectrum of 8-fluoro-6-methyl-5*H*-dibenzo[*b*,*e*][1,4]diazepine (**4af**) in $CDCl_3$.

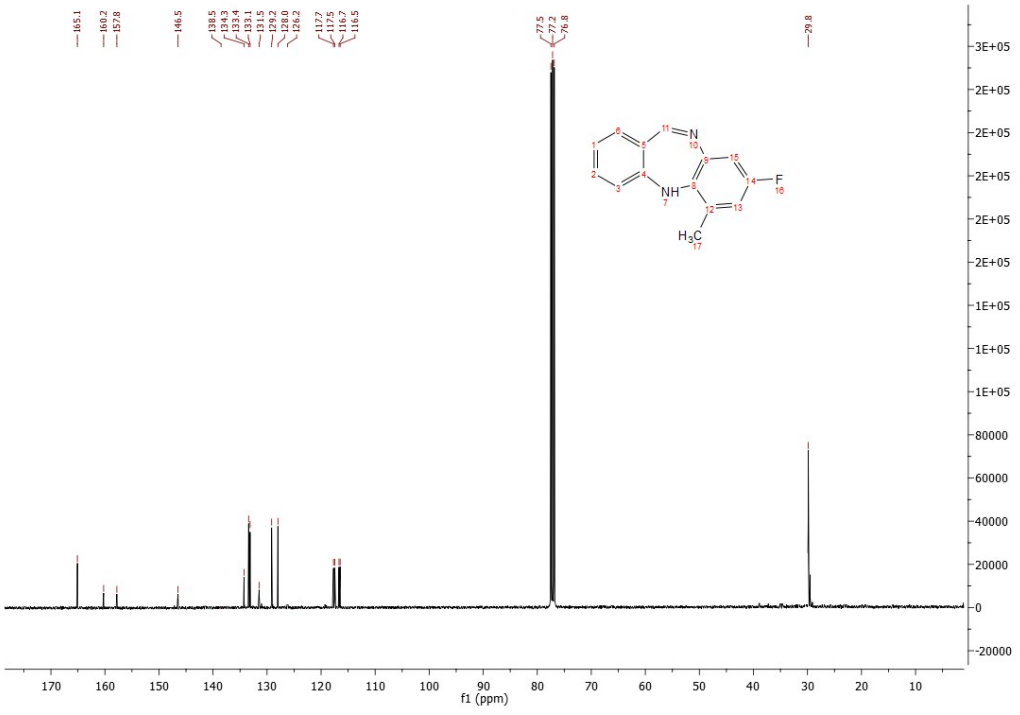


Figure S34. ^{13}C NMR spectrum of 8-fluoro-6-methyl-5*H*-dibenzo[*b*,*e*][1,4]diazepine (**4af**) in $CDCl_3$.

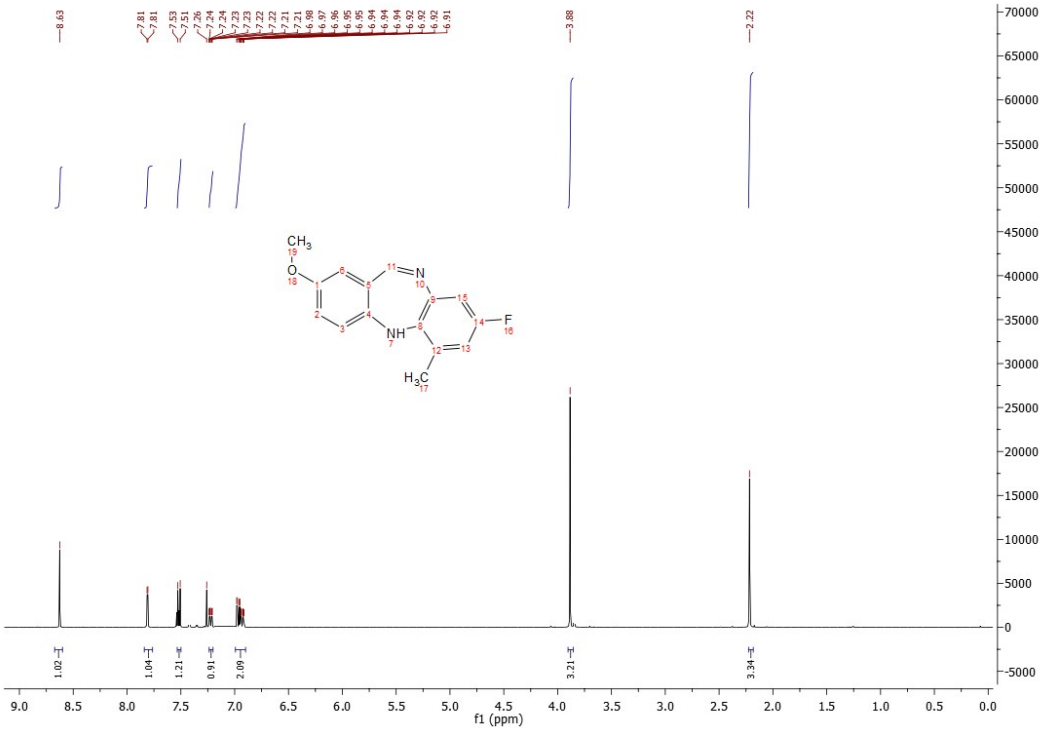


Figure S35. ^{1}H NMR spectrum of 8-fluoro-2-methoxy-6-methyl-5*H*-dibenzo[b,e][1,4]diazepine (**4ef**) in $CDCl_3$.

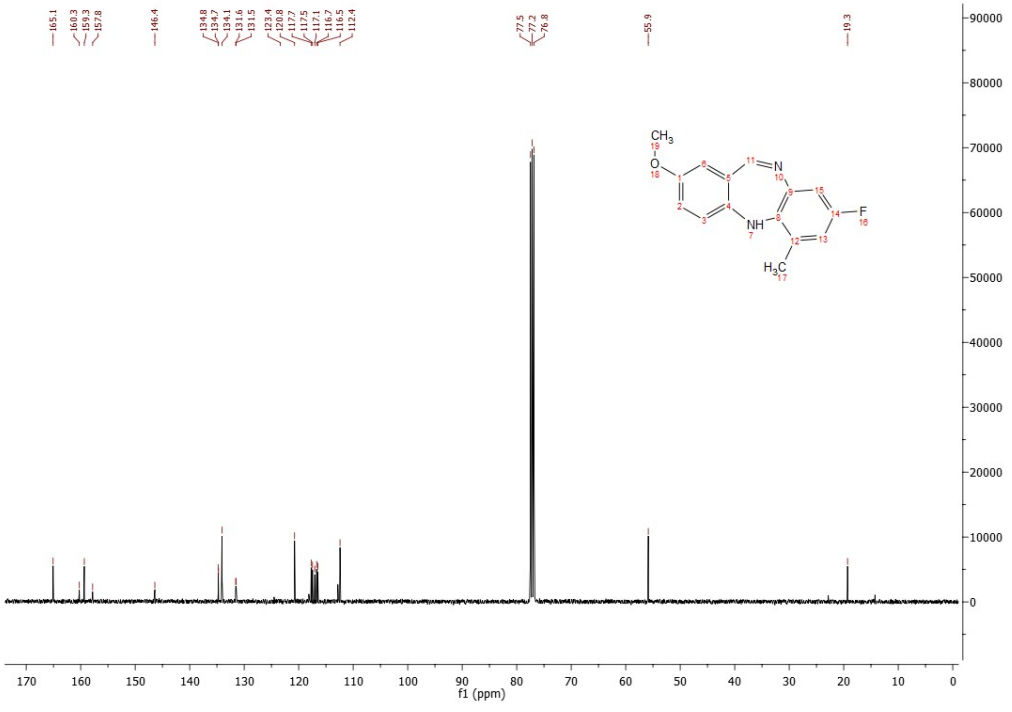


Figure S36. ^{13}C NMR spectrum of 8-fluoro-2-methoxy-6-methyl-5*H*-dibenzo[b,e][1,4]diazepine (**4ef**) in $CDCl_3$.

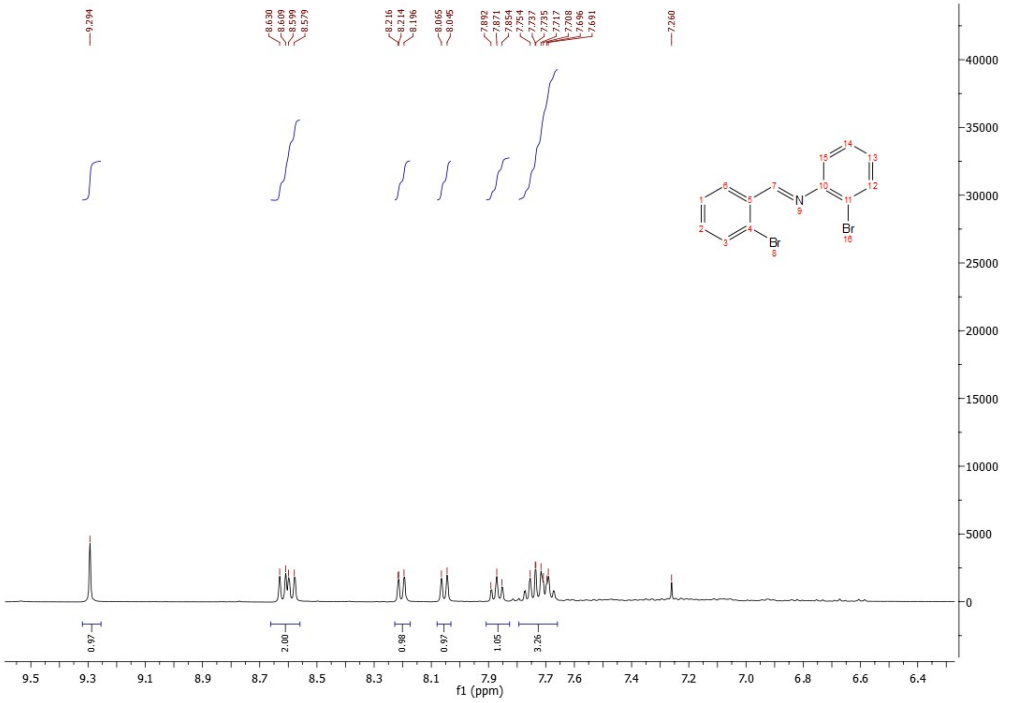


Figure S37. ^{1}H NMR spectrum of (*E*)-2-bromo-*N*-(2-bromobenzylidene)aniline (**5**) in $CDCl_3$.

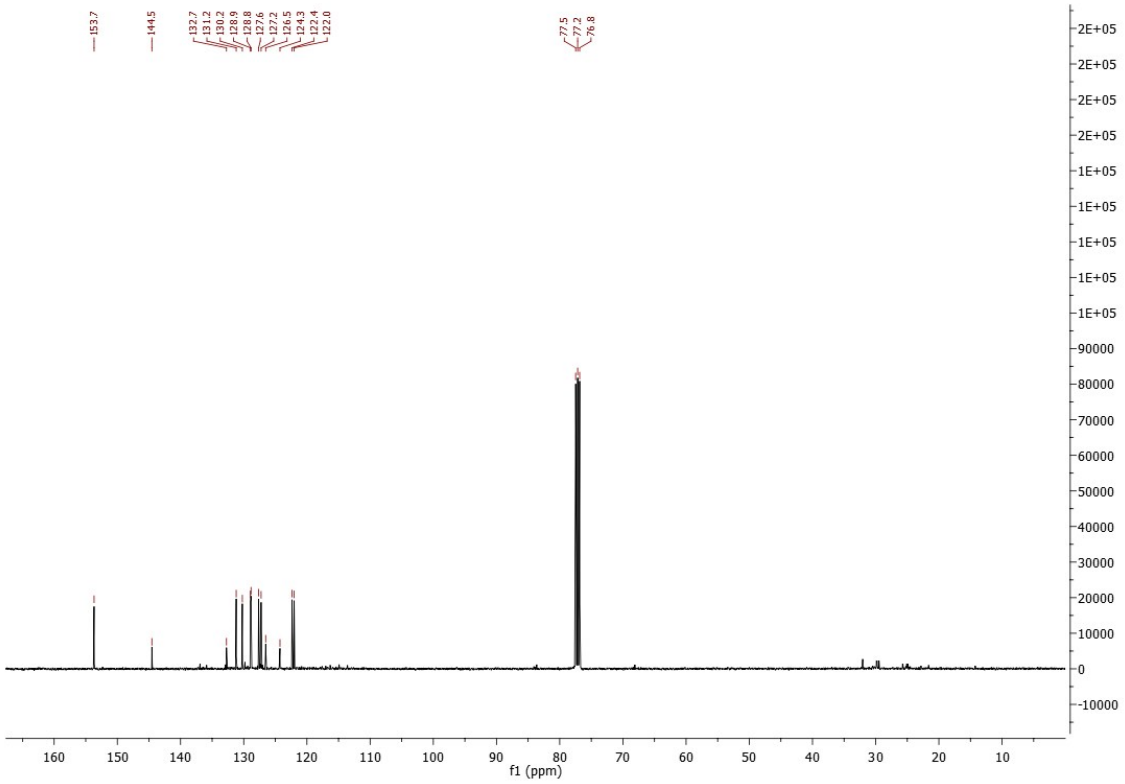


Figure S38. ^{13}C NMR spectrum of (*E*)-2-bromo-*N*-(2-bromobenzylidene)aniline (**5**) in $CDCl_3$.

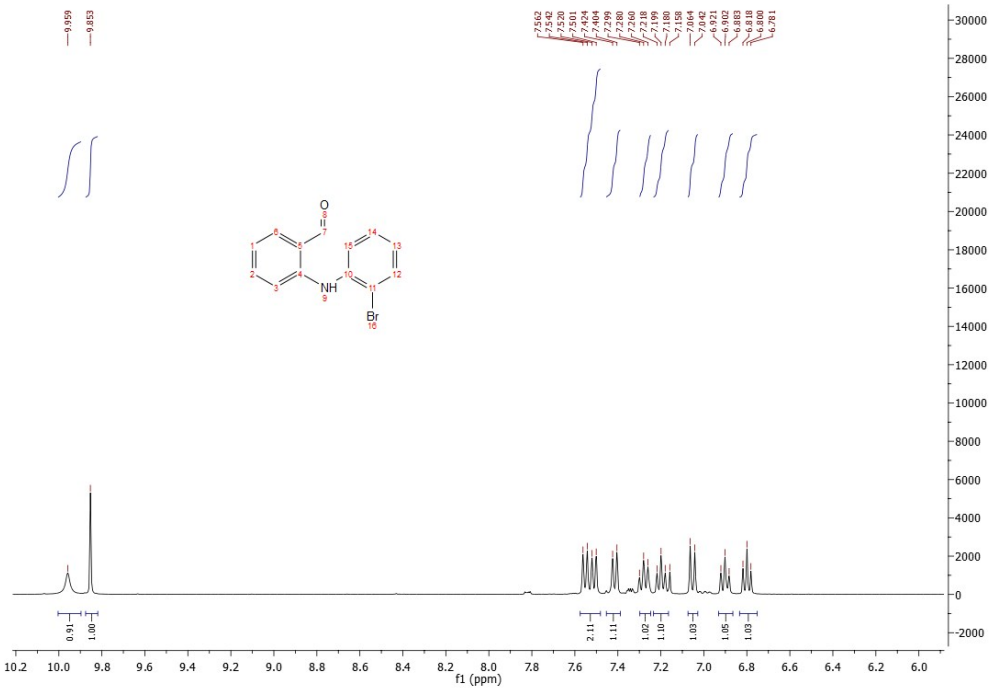


Figure S39. ^{1}H NMR spectrum of 2-(2-bromophenylamino)benzaldehyde (**6**) in $CDCl_3$.

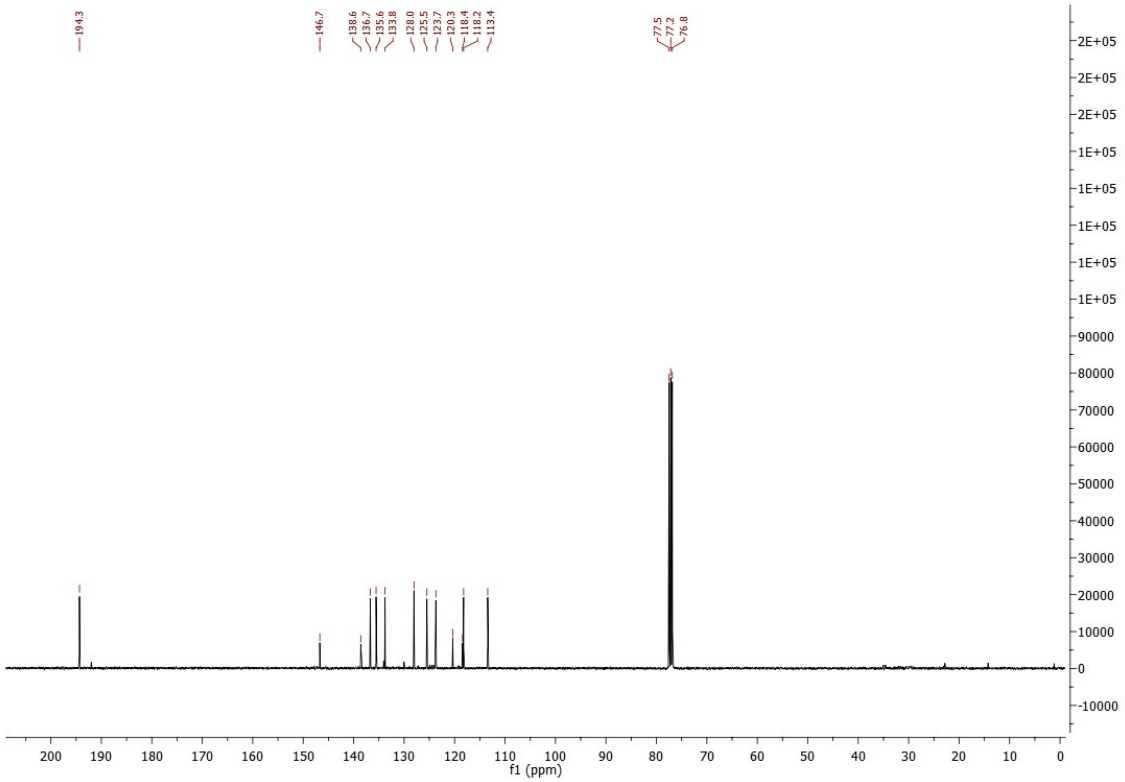
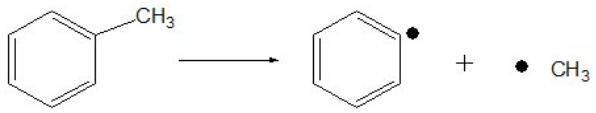


Figure S40. ^{13}C NMR spectrum of 2-(2-bromophenylamino)benzaldehyde (**6**) in $CDCl_3$

Bond Dissociation Energy.

We looked at the Bond Dissociation Energy (BDE) of complexes **2a** and **3b**. The BDE is a way to measure the strength of a chemical bond. To calculate the BDE, one has to optimize each fragments (*i.e.* the radicals) obtained after breaking of the bond considered (Scheme S38).



Scheme S38: Representation of an aromatic bond cleavage; formation of two radicals.

We performed calculations (at the exact same level theory as the optimizations) to get the BDE values of the following complexes (**2a** and **3b**) and the values are reported in Figure S39.

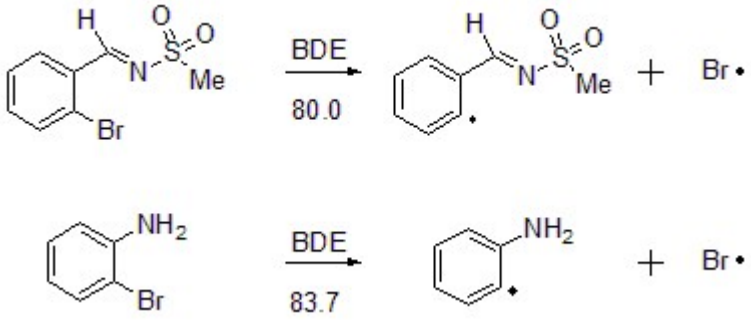


Figure S39: BDE values in kcal/mol, calculated at the DFT (M06) level, for the starting compounds.

Remarkably, we can observe that the C-Br bond of the bromophenyl amine is 3.7 kcal/mol stronger than the corresponding bond for the arylimine. The double bond of the imine is likely to stabilize the radical obtained after the C-Br bond cleavage in the case of **2a**. This is probably due to the fact that the imine, even if located one bond further, is still close enough to the aromatic ring. Aromatization allows the radical to be delocalized as far as the C=N bond. We computed the Mulliken spin density to confirm this hypothesis. The values are collected in Figure S40, and suggest that the radical is indeed delocalized onto the C=N bond. The delocalization does not reach the Ms-group.

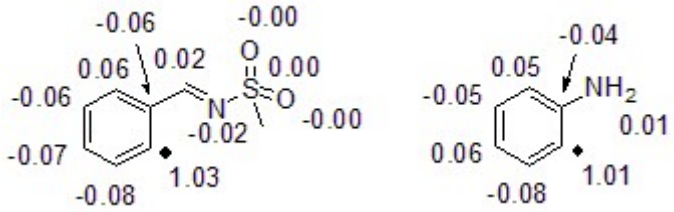


Figure S40: Mulliken spin density values for the radicals obtained from the breaking of the C-Br bonds of **2a** and **3b**.

N-S bond cleavage

We also tested the possibility of N-S bond cleavage in complex **2a**. This is mentioned in the manuscript (the transition state lies too high in energy compared to the oxidation at the C-Br bonds), and a scheme of the transition state is shown here (Figure S41) (Cartesian coordinates are below).

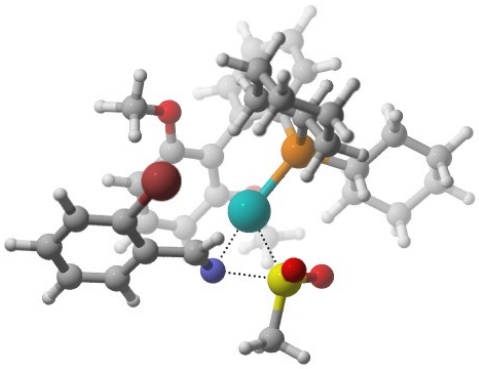


Figure S41: Representation of the transition state for N-S bond cleavage in complex **2a**.

Energetics and Cartesian coordinates.

In the following are the ZPE corrected, and Free Gibbs energies in hartrees for each computed complexes, together with the lowest frequency.

2a_OA_Br_Add
ZPE -2555.967936
Free Gibbs energy -2556.042654
Frequency 20.9368
Pd -0.011358 -0.879892 -0.113024
P 0.545900 1.392093 -0.302483
C 2.599265 -2.780999 -1.486631
C 2.605788 -1.385428 -1.600264
C 3.069522 -0.579047 -0.545193
C 3.500846 -1.204080 0.634318
C 3.508465 -2.595699 0.753031
C 3.071137 -3.363767 -0.318437
O 2.235230 -0.720497 -2.718969
C 3.288999 0.880241 -0.752848
O 3.913290 -0.366506 1.619314
H 3.860416 -3.077386 1.661472
H 3.091142 -4.450356 -0.238130

H 2.248161 -3.405363 -2.303545
C 4.603008 1.273024 -1.030464
C 4.923726 2.596149 -1.297324
C 3.921663 3.559558 -1.291811
C 2.615518 3.185582 -1.005505
C 2.276204 1.854987 -0.725624
H 5.380588 0.509390 -1.044268
H 5.953698 2.872199 -1.517555
H 4.154091 4.600852 -1.509424
H 1.842503 3.953385 -1.004410
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C 1.588484 -1.446993 -3.738778
C -0.485223 2.439986 -1.439225
H -0.133821 3.486629 -1.403047
C 4.081696 -0.903833 2.907236
H 4.937584 -1.593944 2.955328
H 3.172407 -1.430224 3.239754
H 4.271753 -0.055851 3.571561
H 0.682089 -1.943194 -3.358470
H 2.257504 -2.194984 -4.189420
H 1.306438 -0.715317 -4.500136
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C -1.256946 2.700646 -3.830068
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H 0.696695 1.981306 -3.206144
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H -3.896478 3.081188 -1.618521
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C -0.392643 -2.409796 3.220675
C 0.365650 -3.330958 2.471032
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H -4.911484 1.906538 2.371059
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2a_OA_Br_TS

ZPE -2555.958281

Free Gibbs energy -2556.031856

Frequency -100.8273

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C 3.650542 -1.213388 0.459487
C 3.661419 -2.596537 0.261611
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2a_OA_Br_Prod

ZPE -2555.985878

Free Gibbs energy -2556.061892

Frequency 20.2006

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C -0.792356 -0.726799 -2.754386
C 0.696748 0.199425 -4.424305
C -0.573318 -0.230844 -4.036139
Br -0.057623 -3.735539 -0.602334
H -1.786000 -1.062503 -2.467307
H 2.758820 0.389298 -3.810806
H 0.865796 0.586019 -5.427394
H -1.407049 -0.193173 -4.738719
N 3.764759 0.147502 -1.540302
H 2.603661 -1.255739 -0.508705
S 5.060115 -0.163713 -0.493681
O 6.182191 -0.598339 -1.309182
O 4.651619 -0.954521 0.666042
C 5.374142 1.503395 0.051236
H 6.259387 1.469373 0.693960
H 5.562364 2.127243 -0.826859
H 4.509308 1.873078 0.613939

3b_OA_Br_Add

ZPE -1930.170859

Free Gibbs energy -1930.241902

Frequency 20.6882

Pd -1.067648 -0.009976 0.148672
P 1.075141 0.880052 -0.069926
C -1.035387 -2.834424 -1.901601
C 0.035896 -1.950406 -2.067759
C 1.196826 -2.076247 -1.290581
C 1.260137 -3.101512 -0.339208
C 0.193065 -3.985222 -0.155704
C -0.938544 -3.841438 -0.950033
O 0.056838 -0.955907 -2.986368
C 2.367017 -1.189059 -1.526066
O 2.415264 -3.164117 0.374191
H 0.249031 -4.783910 0.579414
H -1.769091 -4.535904 -0.825522
H -1.937781 -2.737044 -2.498478
C 3.438329 -1.729702 -2.244201
C 4.566514 -0.978206 -2.539202
C 4.637064 0.343960 -2.116556
C 3.583728 0.889530 -1.394277
C 2.440194 0.143354 -1.077810
H 3.368488 -2.765970 -2.574674
H 5.385933 -1.422769 -3.102022
H 5.510540 0.952100 -2.347361
H 3.657947 1.927966 -1.074055
C 1.810360 0.982734 1.650657
C -1.141301 -0.649200 -3.660256
C 1.037458 2.647190 -0.652871
H 2.052363 3.079332 -0.604359
C 2.457686 -4.023900 1.482482
H 2.397947 -5.081989 1.184338
H 1.644010 -3.806711 2.192956
H 3.419390 -3.846330 1.973026
H -1.937570 -0.374418 -2.950131
H -1.478878 -1.487111 -4.289037
H -0.916674 0.206600 -4.302350
C 0.123522 3.496872 0.233839
C 0.557547 2.696218 -2.106543
C 0.488511 4.131070 -2.617265
H -0.448254 2.240782 -2.152073
H 1.203988 2.079017 -2.749390
C 0.043489 4.932334 -0.278783
H 0.473710 3.492301 1.277426
H -0.884758 3.044451 0.243831
H -0.630210 5.522500 0.358961
C -0.414893 4.981377 -1.731722
H 1.039880 5.401516 -0.198132
H 0.135827 4.146820 -3.658605
H 1.503898 4.564218 -2.624766
H 1.000010 1.472179 2.225311
H -0.444891 6.019979 -2.091379
H -1.446619 4.594936 -1.796704
C 3.093440 1.794332 1.821673
C 1.986447 -0.422899 2.230235
C 3.501900 1.858535 3.292058
H 2.977653 2.813444 1.419812
H 3.903141 1.314581 1.245156

C 2.407786 -0.364985 3.694971
H 2.747497 -0.968315 1.643749
H 1.044478 -0.985145 2.124547
H 4.427474 2.441875 3.403012
C 3.675483 0.462258 3.876916
H 2.722367 2.396450 3.859101
H 2.550920 -1.381636 4.091373
H 1.589394 0.087032 4.282962
H 3.952802 0.520261 4.939376
H 4.510964 -0.041492 3.360686
C -3.068371 -0.328110 0.883205
C -3.310502 0.792297 1.731333
C -2.409384 -1.482093 1.367133
C -2.844018 0.708400 3.048150
N -3.971176 1.918406 1.283881
C -1.968248 -1.520929 2.700690
H -2.360815 -2.373590 0.742170
C -2.196857 -0.431201 3.527029
H -3.016380 1.559014 3.708871
H -1.468075 -2.415200 3.068903
Br -4.181678 -0.503424 -0.751970
H -1.872355 -0.457170 4.566193
H -4.409657 2.482349 1.999228
H -4.532175 1.808723 0.448183

3b_OA_Br_TS

ZPE -1930.164004

Free Gibbs energy -1930.232652

Frequency -101.7378

Pd -0.988025 0.663636 -0.419690
P 1.250593 0.480113 0.269542
C -1.309604 -1.466322 -3.158866
C -0.010799 -1.185628 -2.720806
C 0.599762 -1.971951 -1.732004
C -0.120039 -3.042681 -1.186864
C -1.412214 -3.342177 -1.625880
C -1.985844 -2.550187 -2.612530
O 0.752786 -0.183161 -3.218461
C 2.017352 -1.738434 -1.343536
O 0.525215 -3.747667 -0.221370
H -1.965230 -4.177329 -1.203289
H -2.992446 -2.778111 -2.962054
H -1.789312 -0.852112 -3.915734
C 2.960232 -2.623495 -1.877081
C 4.315607 -2.487713 -1.615875
C 4.753510 -1.446857 -0.805847
C 3.827045 -0.567272 -0.261109
C 2.452488 -0.692683 -0.506933
H 2.604684 -3.432097 -2.515521
H 5.027661 -3.189339 -2.047752
H 5.814176 -1.316961 -0.595820
H 4.191303 0.242162 0.370109
C 1.226513 -0.034276 2.069355
C 0.140952 0.752656 -4.074029
C 2.172945 2.097313 0.259101
H 3.174870 1.964499 0.703672
C -0.233172 -4.635812 0.559463
H -0.596124 -5.493339 -0.027754
H -1.091905 -4.125470 1.025023
H 0.435918 -5.002254 1.343679
H -0.716956 1.237199 -3.581283
H -0.186852 0.288055 -5.016270
H 0.902152 1.505786 -4.294096
C 1.425353 3.146514 1.084828
C 2.338705 2.576715 -1.185878
C 3.042225 3.927946 -1.248177
H 1.332381 2.664092 -1.634162
H 2.876850 1.824035 -1.782201
C 2.124558 4.501474 1.016519
H 1.328942 2.825182 2.132942
H 0.395099 3.233281 0.694328
H 1.562898 5.244211 1.601183
C 2.294461 4.969495 -0.423955
H 3.119227 4.419392 1.488722
H 3.138289 4.256961 -2.292935
H 4.069453 3.823817 -0.857578
H 0.539366 0.705803 2.522348
H 2.815444 5.937152 -0.456128
H 1.298195 5.132484 -0.869814
C 2.552527 0.001381 2.827464
C 0.565987 -1.408437 2.209970
C 2.344770 -0.356324 4.297815
H 3.032053 0.989767 2.746976
H 3.247341 -0.727319 2.375877
C 0.372973 -1.777270 3.676984
H 1.195798 -2.168713 1.714052
H -0.404159 -1.411634 1.687271
H 3.304849 -0.327228 4.833244
C 1.689136 -1.724250 4.444298
H 1.700625 0.407779 4.766694
H -0.087624 -2.773917 3.759542
H -0.342638 -1.068151 4.129552
H 1.530709 -1.964363 5.505626
H 2.372778 -2.493541 4.045536
C -2.835739 0.354495 0.601566
C -2.813335 0.893723 1.906623
C -3.147146 -0.985451 0.363000
C -2.994646 -0.008670 2.961362
N -2.552623 2.231713 2.157567
C -3.321126 -1.854741 1.437320
H -3.217746 -1.342150 -0.663442
C -3.242278 -1.358597 2.735396
H -2.932144 0.374668 3.981468
H -3.538630 -2.905916 1.251564
Br -3.329512 1.696300 -0.990198

H -3.386319 -2.022520 3.586452
H -2.984478 2.599205 2.996220
H -2.657913 2.847250 1.358823
3b_OA_Br_Prod
ZPE -1930.199412
Free Gibbs energy -1930.269185
Frequency 14.5622
Pd -0.939770 -1.002862 -0.160726
P 0.162650 1.055999 -0.382570
C 1.378623 -3.498050 -0.244025
C 1.468688 -2.259660 -0.874948
C 2.444481 -1.319169 -0.537847
C 3.322891 -1.637277 0.513885
C 3.226146 -2.856954 1.182254
C 2.263885 -3.780164 0.784613
O 0.540583 -1.845324 -1.810663
C 2.633389 -0.073088 -1.326376
O 4.245115 -0.688679 0.818002
H 3.903357 -3.099291 1.996470
H 2.190772 -4.733137 1.304888
H 0.582091 -4.190734 -0.501830
C 3.816931 -0.003649 -2.071326
C 4.122843 1.091726 -2.863376
C 3.233820 2.156783 -2.920183
C 2.057506 2.105633 -2.184862
C 1.726499 1.005586 -1.379602
H 4.507690 -0.844279 -2.017387
H 5.049261 1.110316 -3.434763
H 3.450859 3.029445 -3.533717
H 1.383108 2.956460 -2.250053
C 0.662536 1.965593 1.159761
C 0.097492 -2.802569 -2.771244
C -0.921556 2.228694 -1.326957
H -0.335234 3.134836 -1.555357
C 4.944572 -0.817747 2.031390
H 5.653983 -1.658507 2.009407
H 4.250365 -0.954581 2.874632
H 5.499936 0.114738 2.166319
H -0.559012 -3.553598 -2.317225
H 0.968227 -3.275376 -3.243462
H -0.471804 -2.234531 -3.512511
C -2.145386 2.681793 -0.527567
C -1.351146 1.589166 -2.652026
C -2.199788 2.556666 -3.470490
H -1.935476 0.678006 -2.430989
H -0.470608 1.263886 -3.228542
C -2.966831 3.669947 -1.351776
H -1.847131 3.135456 0.429986
H -2.774810 1.812581 -0.291012
H -3.842492 3.996309 -0.773497
C -3.403461 3.044824 -2.672085
H -2.367980 4.576113 -1.554292
H -2.522405 2.075414 -4.404590
H -1.580054 3.422860 -3.763121
H -0.252060 1.953090 1.780733
H -3.993012 3.759566 -3.263698
H -4.063592 2.188084 -2.456127
C 1.093490 3.417727 0.941807
C 1.757670 1.207055 1.916490
C 1.386553 4.093988 2.279772
H 0.320531 3.985065 0.402496
H 2.000615 3.435990 0.312523
C 2.025964 1.871563 3.262828
H 2.681962 1.208294 1.313679
H 1.483955 0.149235 2.053873
H 1.708786 5.131672 2.112914
C 2.435429 3.327951 3.076807
H 0.452659 4.145783 2.864918
H 2.804351 1.322083 3.812329
H 1.110167 1.818223 3.877393
H 2.605552 3.810376 4.049735
H 3.396841 3.362401 2.535605
C -1.990732 -0.345674 1.414403
C -3.352636 -0.011465 1.322333
C -1.347283 -0.293077 2.646224
C -3.994603 0.474010 2.469825
N -4.044900 -0.092433 0.108830
C -2.003031 0.173489 3.787081
H -0.310876 -0.622599 2.725517
C -3.329630 0.574652 3.685352
H -5.046626 0.757745 2.397230
H -1.478163 0.211529 4.740772
Br -2.321097 -3.123699 -0.144937
H -3.861904 0.947810 4.559286
H -5.051147 -0.120762 0.238139
H -3.743854 -0.895609 -0.443254
cycl_CN_noMs_Add
ZPE -2240.314579
Free Gibbs energy -2240.388557
Frequency 10.1914
N 3.954033 0.219259 0.759332
C 3.794064 1.487739 0.205713
C 3.676391 2.524063 1.153448
C 3.830152 1.847078 -1.163567
C 3.623241 3.859977 0.797199
H 3.627328 2.246896 2.208799
C 3.794451 3.209641 -1.490531
C 3.843601 0.958043 -2.364584
C 3.685220 4.219266 -0.545876
H 3.533711 4.618709 1.573251
H 3.848747 3.468581 -2.549317
H 3.655982 5.263377 -0.851195
H 4.570856 1.298988 -3.129997
N 3.057574 0.017795 -2.688590

H 2.121330 -3.168534 -1.793114
C 2.829907 -2.856970 -1.025259
C 3.641308 -3.809291 -0.411308
H 3.566366 -4.856910 -0.699231
C 4.546861 -3.405685 0.564781
H 5.191180 -4.132234 1.057284
C 4.655212 -2.060838 0.889580
H 5.393971 -1.733433 1.624536
C 3.837137 -1.095898 0.281171
C 2.876505 -1.519112 -0.642453
H 4.318083 0.260121 1.702863
H -6.503982 -1.315938 1.245510
H -2.808049 -0.746507 4.100310
H -4.873260 -0.857935 3.033962
H -3.917960 0.619788 4.452633
C -5.670771 -0.642834 1.050603
C -4.749405 -0.393746 2.059676
C -2.932672 0.347768 4.046365
H -2.152371 0.825007 4.646112
H -6.312560 -0.232148 -0.958307
C -5.565204 -0.036195 -0.194384
C -3.682618 0.471355 1.801367
O -2.764573 0.825801 2.735300
H -5.396531 0.309707 -2.982657
C -4.483036 0.811661 -0.445409
C -3.500630 1.037263 0.531957
P -0.434252 -0.356175 -0.061505
H -6.254252 1.699408 -2.242566
C -5.283372 1.341291 -2.616413
O -4.284971 1.441143 -1.630025
H -4.958352 1.977475 -3.443540
C -2.324413 1.897662 0.233658
C -1.024518 1.406708 -0.023346
H -3.563841 3.633471 0.386094
C -2.551220 3.276175 0.198973
C -0.009294 2.342190 -0.285347
H 1.010173 1.990026 -0.468815
C -1.531475 4.181862 -0.061411
C -0.248010 3.710788 -0.301336
H -1.742634 5.250020 -0.075702
H 0.574855 4.394323 -0.504156
C -1.836769 -1.355436 -0.764364
C -2.030813 -0.923287 -2.223334
C -1.600210 -2.864394 -0.684308
H -2.751649 -1.133042 -0.195179
C -3.158809 -1.699976 -2.892014
H -1.087585 -1.110735 -2.770106
H -2.222312 0.157763 -2.284960
C -2.730102 -3.631422 -1.367245
H -0.635353 -3.116671 -1.159948
H -1.534353 -3.184960 0.364263
C -2.909828 -3.200058 -2.816684
H -3.275820 -1.371251 -3.935219
H -4.107819 -1.470004 -2.375314
H -2.539694 -4.712089 -1.301833
H -3.669040 -3.442322 -0.816628
H -3.734020 -3.755934 -3.286031
H -1.997798 -3.446544 -3.386723
C -0.220165 -0.847965 1.734598
C 0.616205 -2.128021 1.861689
C 0.471636 0.292980 2.490961
H -1.225865 -1.011803 2.165758
C 0.882562 -2.492580 3.317693
H 1.582652 -1.964693 1.363702
H 0.149155 -2.972814 1.339994
C 0.789698 -0.077371 3.936709
H 1.416906 0.528396 1.968169
H -0.145336 1.201214 2.461945
C 1.606688 -1.358214 4.027995
H 1.475323 -3.417755 3.358451
H -0.070715 -2.700710 3.836633
H 1.312999 0.758698 4.424318
H -0.152452 -0.222421 4.494017
H 1.811447 -1.615053 5.077299
H 2.586523 -1.204033 3.541757
Pd 1.521084 -0.282676 -1.452646
cycl_CN_noMs_TS
ZPE -2240.307455
Free Gibbs energy -2240.379779
Frequency -352.7666
N 3.823986 0.353801 0.896139
C 3.771506 1.608310 0.304041
C 3.663678 2.687485 1.198732
C 3.857988 1.899468 -1.079658
C 3.659609 4.005758 0.774531
H 3.580619 2.465639 2.264484
C 3.877725 3.243705 -1.473286
C 3.890459 0.943320 -2.215962
C 3.769911 4.299929 -0.580756
H 3.572676 4.802760 1.511676
H 3.967689 3.451103 -2.540590
H 3.778234 5.328298 -0.935019
H 4.491279 1.325813 -3.063244
N 3.291555 -0.161134 -2.433811
H 2.782385 -2.919967 -2.164004
C 3.272281 -2.652028 -1.228446
C 3.956288 -3.614155 -0.486728
H 3.985632 -4.646488 -0.831674
C 4.606396 -3.241358 0.683929
H 5.154492 -3.975031 1.272317
C 4.587281 -1.909853 1.088135
H 5.129878 -1.602741 1.984988
C 3.881587 -0.943285 0.364372
C 3.169514 -1.340203 -0.774248

H 4.026247 0.391734 1.887305
H -6.604781 -1.359173 0.807586
H -3.014902 -1.378065 3.855225
H -5.058204 -1.241597 2.722395
H -4.124810 -0.080857 4.409262
C -5.751491 -0.684251 0.765913
C -4.878915 -0.625872 1.845631
C -3.126794 -0.290507 3.996805
H -2.367420 0.058068 4.702604
H -6.281012 0.066919 -1.179505
C -5.571983 0.114277 -0.357116
C -3.785198 0.242471 1.784411
O -2.902236 0.412269 2.800657
H -5.135409 0.805650 -3.035611
C -4.464925 0.965735 -0.409677
C -3.531838 1.003995 0.637057
P -0.480695 -0.321199 -0.157548
H -6.095014 2.095512 -2.240440
C -5.083039 1.790517 -2.546414
O -4.194087 1.782718 -1.457061
H -4.687510 2.520845 -3.256893
C -2.331190 1.875566 0.529001
C -1.049624 1.419117 0.152473
H -3.525854 3.568607 1.057379
C -2.525252 3.236324 0.780226
C -0.021595 2.368568 0.037317
H 0.974568 2.032281 -0.262584
C -1.489221 4.154901 0.677547
C -0.226770 3.717015 0.300736
H -1.673227 5.208424 0.883413
H 0.602308 4.415987 0.200204
C -1.897245 -1.233725 -0.953879
C -2.099508 -0.674294 -2.366636
C -1.659861 -2.745016 -1.004101
H -2.809769 -1.063802 -0.364469
C -3.221318 -1.399330 -3.103139
H -1.155101 -0.798403 -2.928011
H -2.304897 0.405841 -2.326783
C -2.791003 -3.451883 -1.746033
H -0.694950 -2.955167 -1.501953
H -1.589337 -3.153425 0.013716
C -2.966786 -2.899897 -3.153971
H -3.335003 -0.985671 -4.116464
H -4.175479 -1.218125 -2.575299
H -2.603109 -4.534751 -1.771252
H -3.730264 -3.305967 -1.182836
H -3.787116 -3.416326 -3.672851
H -2.051087 -3.094111 -3.738241
C -0.273038 -1.053896 1.561624
C 0.628996 -2.294169 1.515842
C 0.330204 -0.011948 2.511010
H -1.276748 -1.336887 1.928293
C 0.878760 -2.872746 2.903633
H 1.595516 -2.005928 1.076816
H 0.221873 -3.066063 0.850376
C 0.639090 -0.594950 3.887853
H 1.264969 0.372878 2.060120
H -0.348744 0.844942 2.617084
C 1.522826 -1.831600 3.807272
H 1.518356 -3.763188 2.819600
H -0.075105 -3.205877 3.351659
H 1.097753 0.177792 4.522519
H -0.307456 -0.878684 4.380065
H 1.709758 -2.240698 4.810753
H 2.507474 -1.559034 3.386641
Pd 1.515604 -0.302448 -1.414757

cycl_CN_noMs_Prod

ZPE -2240.376643

Free Gibbs energy -2240.449343

Frequency 15.7188

N 4.362553 0.674359 0.668068
C 3.923386 1.832996 0.048948
C 4.003115 3.013593 0.798182
C 3.402991 1.897784 -1.259382
C 3.597790 4.236551 0.281221
H 4.396834 2.962672 1.814670
C 3.013481 3.145914 -1.759411
C 3.182624 0.753707 -2.153817
C 3.102315 4.314676 -1.015543
H 3.676104 5.129345 0.899304
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H 2.787112 5.265481 -1.440292
H 2.856760 1.061618 -3.154506
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H 3.832523 -2.951999 -2.130164
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C 4.614445 -3.446566 -0.176395
H 4.680950 -4.514502 -0.372197
C 4.998365 -2.917458 1.048787
H 5.375148 -3.559616 1.842956
C 4.903423 -1.548550 1.263805
H 5.206318 -1.137069 2.229092
C 4.424447 -0.667271 0.287021
C 4.036827 -1.197750 -0.965488
H 4.693511 0.829504 1.611847
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H -2.912370 -1.225573 3.966274
H -4.991522 -1.214474 2.916668
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C -5.783075 -0.801751 0.962209
C -4.868535 -0.649548 1.997091
C -3.039530 -0.133735 4.043847
H -2.257272 0.272086 4.691831
H -6.412974 -0.198840 -1.001370

C -5.672741 -0.074734 -0.216033
C -3.805899 0.243383 1.833809
O -2.884288 0.495734 2.797431
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C -4.594647 0.801539 -0.371828
C -3.624173 0.938802 0.631335
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H -6.325476 1.728916 -2.233304
C -5.310803 1.435470 -2.542179
O -4.392995 1.551703 -1.482963
H -4.961980 2.116937 -3.322198
C -2.462059 1.845272 0.423862
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H -3.697400 3.516100 0.930143
C -2.696235 3.208391 0.627381
C -0.193107 2.399175 -0.177895
H 0.799161 2.085941 -0.510327
C -1.698239 4.157542 0.452913
C -0.435546 3.748174 0.045731
H -1.911921 5.211134 0.627802
H 0.367241 4.468540 -0.108874
C -1.958617 -1.373732 -0.783775
C -2.316552 -1.002449 -2.226084
C -1.617667 -2.861943 -0.687695
H -2.827536 -1.190923 -0.134799
C -3.451752 -1.869673 -2.762642
H -1.417387 -1.141378 -2.852710
H -2.581325 0.063465 -2.293601
C -2.765649 -3.716387 -1.219013
H -0.699364 -3.069872 -1.267742
H -1.405393 -3.139368 0.354973
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H -3.675346 -1.596446 -3.805111
H -4.367074 -1.670177 -2.176165
H -2.509575 -4.782744 -1.139464
H -3.653679 -3.555594 -0.581840
H -3.945663 -3.968026 -3.021297
H -2.247261 -3.573024 -3.304936
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C 0.917769 -1.986924 1.502997
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C 1.307975 -2.465417 2.896917
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C 0.720355 -0.219080 3.814557
H 1.182347 0.752680 1.944344
H -0.470900 1.028468 2.509255
C 1.790070 -1.299993 3.749135
H 2.088106 -3.236150 2.812890
H 0.440648 -2.942251 3.387611
H 1.059518 0.633400 4.421498
H -0.165611 -0.634762 4.327518
H 2.065518 -1.637530 4.758918
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CN_noMs_Add

ZPE -2240.314402

Free Gibbs energy -2240.387505

Frequency 18.1369

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H 3.648150 5.258794 -0.961353
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C 3.651692 -3.792167 -0.324914
H 3.596376 -4.844464 -0.599840
C 4.518735 -3.366084 0.676502
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C 4.604578 -2.015317 0.983946
H 5.315682 -1.669964 1.737884
C 3.800109 -1.067132 0.332492
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H 4.226134 0.319907 1.742588
H -6.470327 -1.309526 1.421671
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C -5.575344 -0.059050 -0.071003
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O -2.696840 0.872713 2.759741
H -5.495028 0.235064 -2.865355
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O -4.339921 1.391177 -1.572218

H -5.067117 1.890771 -3.375416
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C -0.268651 3.700048 -0.377810
H -1.761416 5.239778 -0.143341
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C -1.854117 -1.360669 -0.783282
C -2.059153 -0.901847 -2.233153
C -1.602716 -2.869052 -0.733201
H -2.766880 -1.155459 -0.203285
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H -1.113684 -1.063051 -2.784708
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C -2.721664 -3.636190 -1.433531
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H -2.518520 -4.715506 -1.387465
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H 0.043243 -2.991328 1.383401
C 0.918347 -0.059643 3.863308
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H 1.489223 -3.423846 3.321342
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H 0.013043 -0.181028 4.483450
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CN_noMs_TS

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Free Gibbs energy -2240.342988

Frequency -457.9024

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C 4.192816 -3.505403 -2.139731
H 3.579112 -1.776310 -3.268727
C 4.520740 -3.129993 0.203654
C 4.115808 -1.039444 1.414637
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H 4.778303 -3.501636 1.196504
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H -3.310931 -2.159253 -3.169428
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H 1.176316 -1.274836 -1.321721
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C -2.792480 1.016630 3.677141
H -0.713871 1.185103 3.091194
H -1.821035 2.230231 2.185323
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CN_noMs_Prod

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Free Gibbs energy -2240.370497

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H 4.782708 3.874472 1.715591
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C -3.582223 -0.717126 -1.045425
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C 0.007893 -2.443772 -2.629224
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H -4.076247 -1.103123 2.853803
H -2.946896 2.192595 4.285846
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H -0.087515 2.992913 1.345112
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Ms_bound_N_Add
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Free Gibbs energy -2828.782268
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Ms_bound_N_TS

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Free Gibbs energy -2828.729423

Frequency -431.2989

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