Supplementary Information

Pyreno-1,2,4-Triazines as Multifunctional Luminogenic Click Reagents

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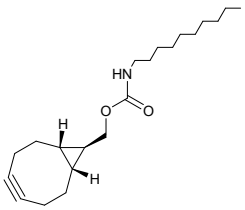
Contents

Synthesis

General

All solvents and reagents were purchased from commercial suppliers and used without further purification. NMR spectra were recorded on a JEOL ECS400FT Delta spectrometer (400 MHz for ^{1}H NMR, 100MHz for ^{13}C NMR). Chemical shifts are reported in parts per million (ppm) relative to a tetramethylsilane internal standard. Infrared spectra were recorded on a Bruker ALPHA Platinum ATR spectrometer and annotated using OPUS 7.0 software. UV-Vis spectra were recorded on a Varian Cary 50 Bio UV-Visible Spectrophotometer. The LC/HRMS analysis of the organic samples were performed on a Thermo scientific Vanquish IDX High Resolution Tribrid Mass Spectrometer system. Northumbria University Metabolomics Core Service. Dienophiles **11**[1] and **12**[2] were prepared as described previously.

Synthesis of BCN derivative 13



To a solution of *anti*-BCN-NHS (750 mg, 2.58 mmol) in DCM (50 mL), triethylamine (800 mkL) and N-decylamine (500 mkL) were added. The mixture was stirred under argon in the dark at RT for 36 hours. Water (50 mL) was added. The mixture was separated. The aqueous layer was washed with DCM (2X25 mL). Combined organic fraction was dried over magnesium sulphate, gravity filtered and evaporated to dryness. The product was purified by column chromatography using silica gel (35 g) as a stationary phase and a mixture of DCM/petrol ether, 4/1, v/v as an eluent (Rf = 0.4). Product is a colourless solid. Yield 620 mg (72%).

^{1}H NMR (400 MHz, $CDCl_3$, Me_4Si) δ: 10.61 (br.s, 1H), 3.95 (d, *J* = 6.5 Hz, 2H), 3.15 (q, *J* = 6.5 Hz, 2H), 2.12–2.44 (m, 6H), 1.48 (quintet, *J* = 6.8 Hz, 2H), 1.21-1.41 (m, 16H), 0.88 (t, *J* = 6.8 Hz, 3H), 0.64-0.78 (m, 2H).
^{13}C NMR (100.6 M, $CDCl_3$, Me_4Si) δ: 156.7, 98.8, 68.9, 41.0, 33.3, 31.9, 30.0, 29.6, 29.3, 26.8, 23.8, 22.8, 22.7, 21.4, 14.1.

Copies of NMR spectra

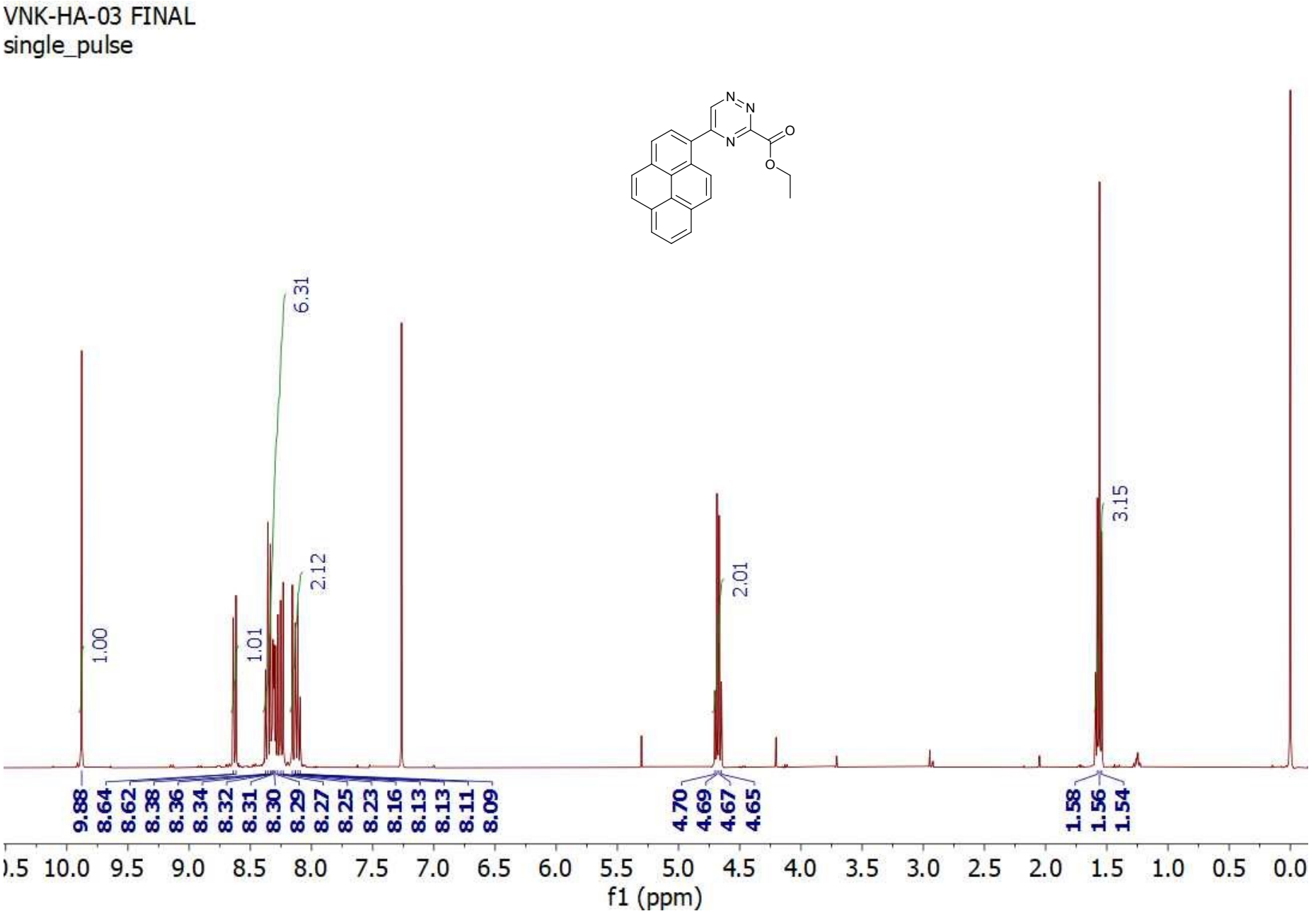


Figure S1. ^{1}H NMR spectrum of **5** in $CDCl_3$

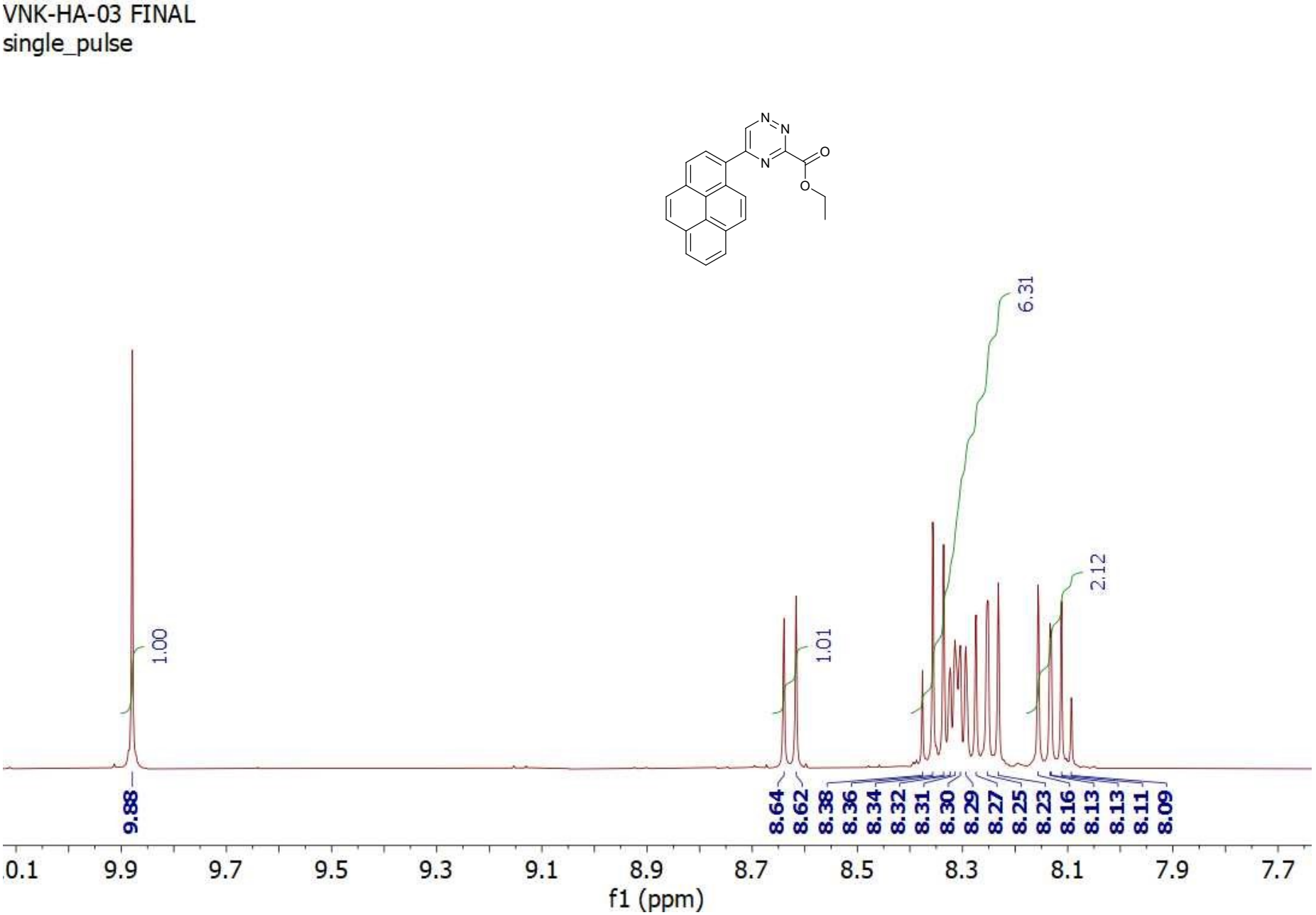


Figure S2. An aromatic region of ^{1}H NMR spectrum of **5** in $CDCl_3$.

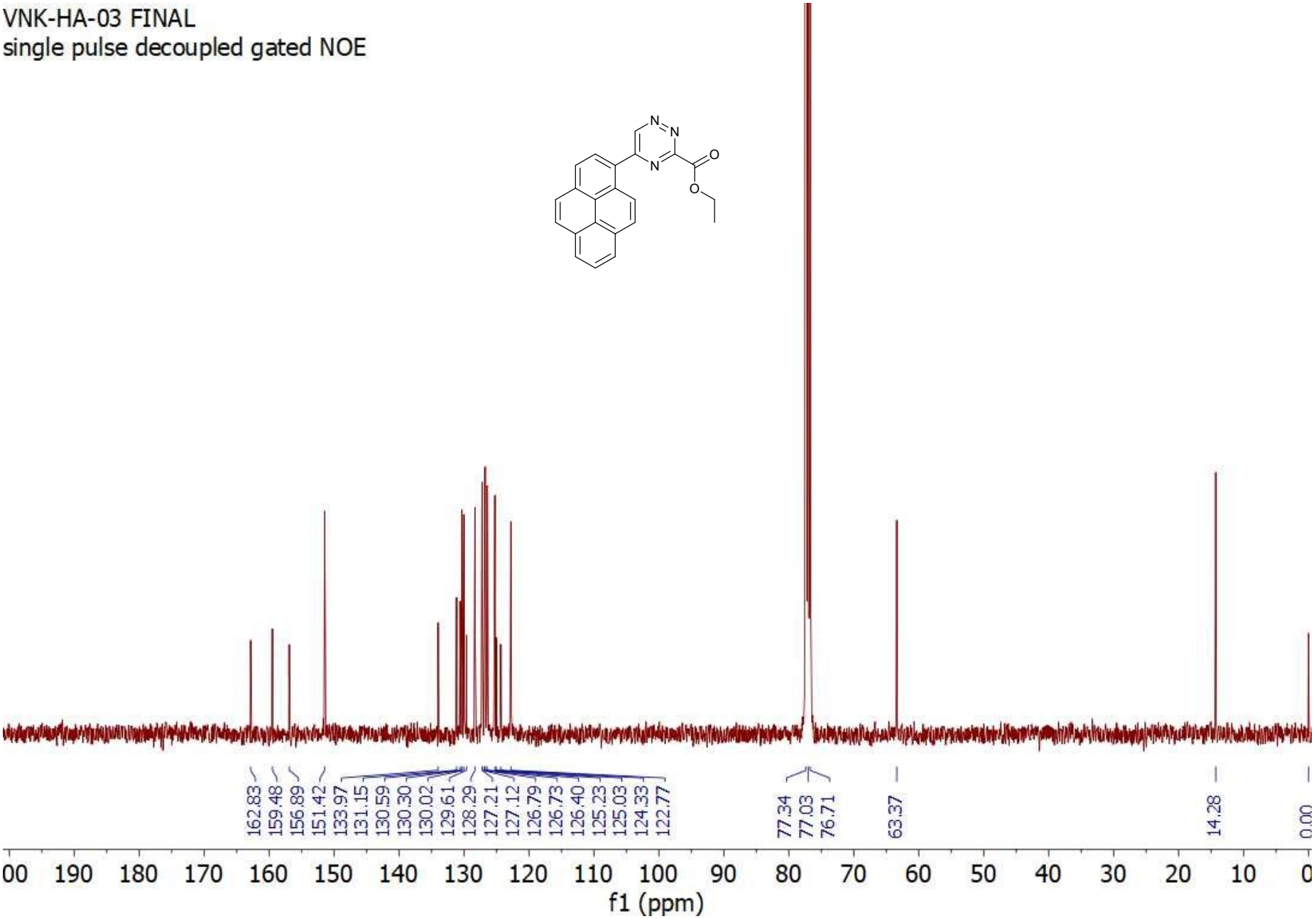


Figure S3. ^{13}C NMR spectrum of **5** in $CDCl_3$

VNK-HA-03 FINAL
single pulse decoupled gated NOE

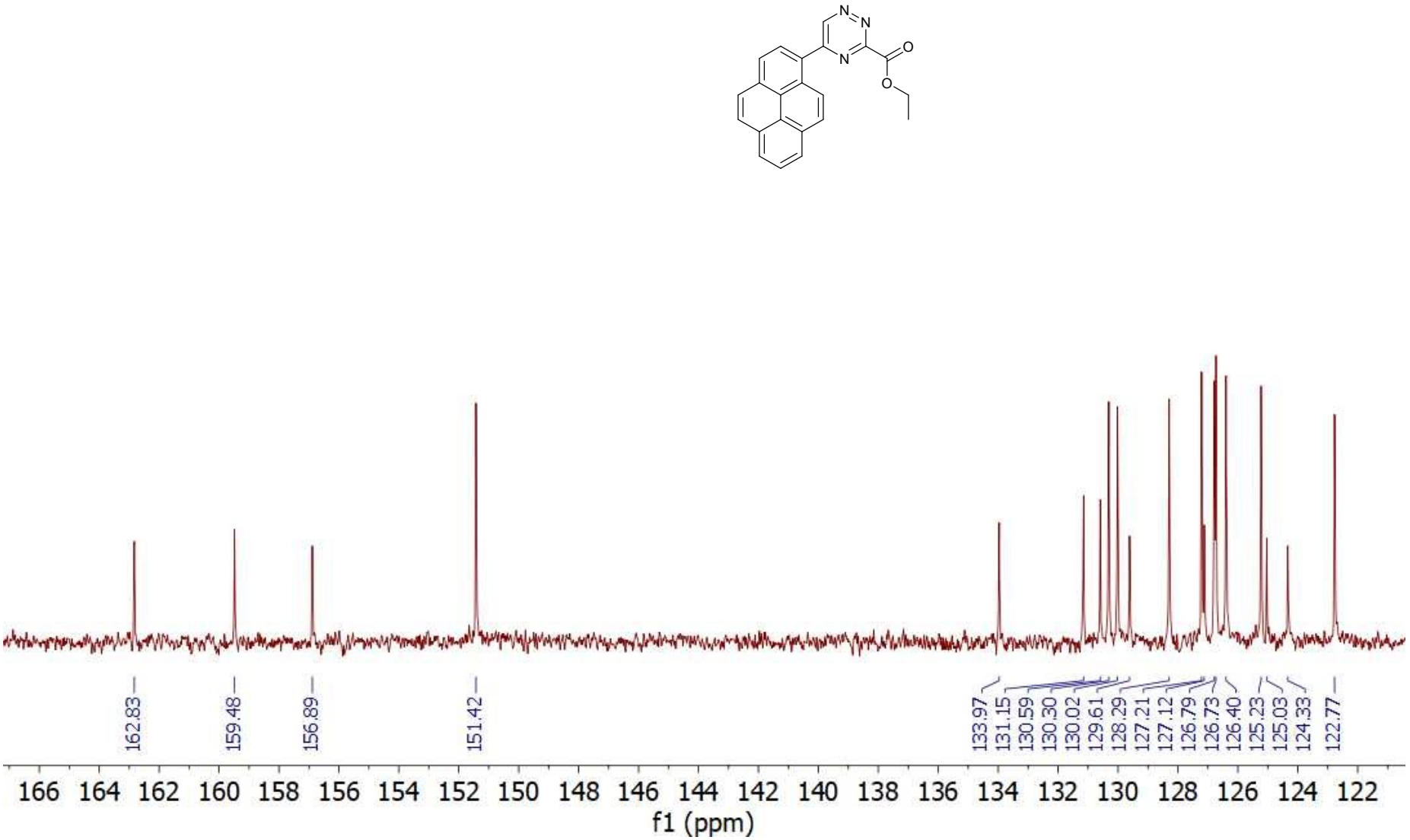


Figure S4. An Aromatic region of ^{13}C NMR spectrum of **VNK-HA-03** in $CDCl_3$

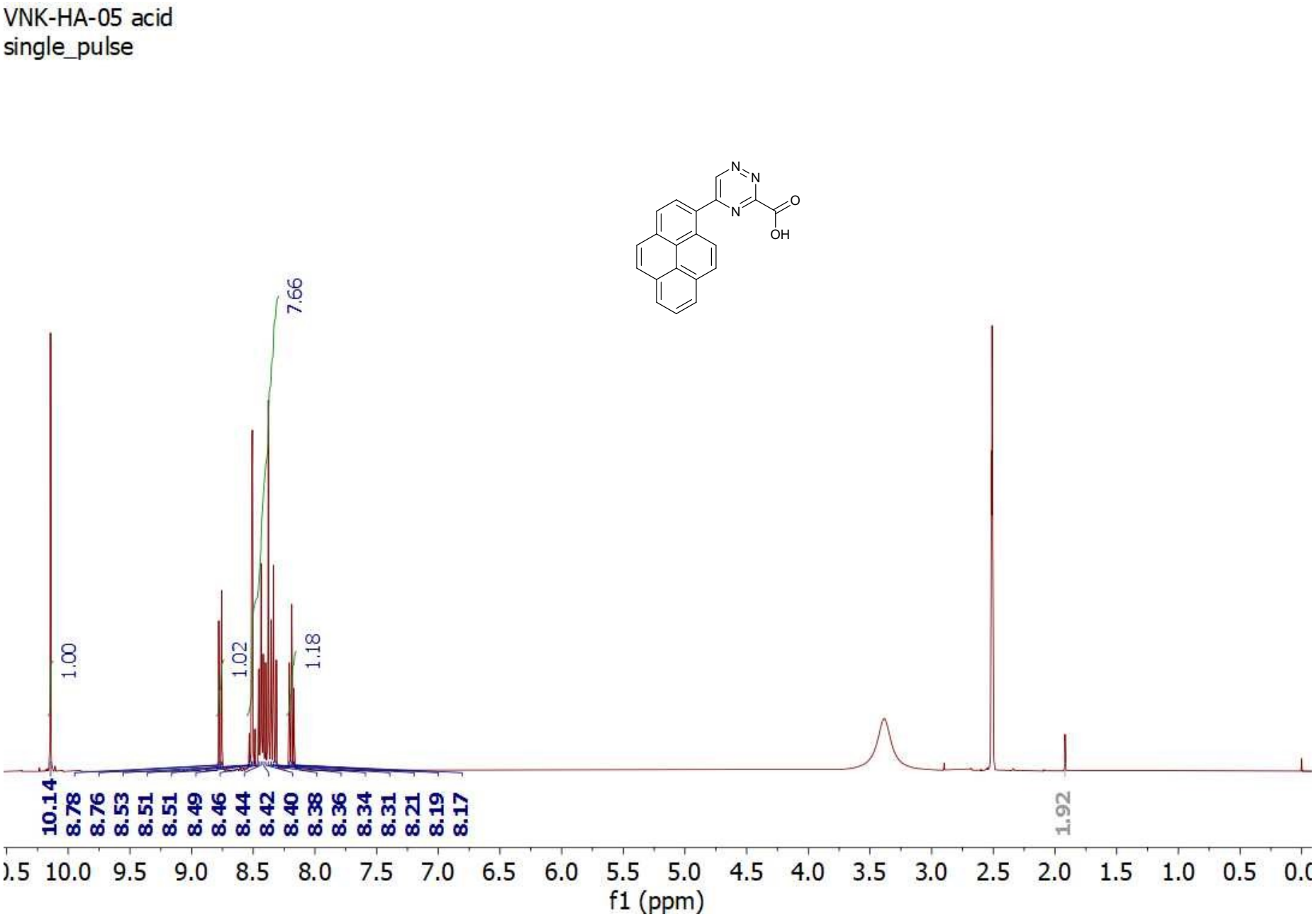


Figure S5. ^{1}H NMR spectrum of **VNK-HA-05 acid** in DMSO-D_6

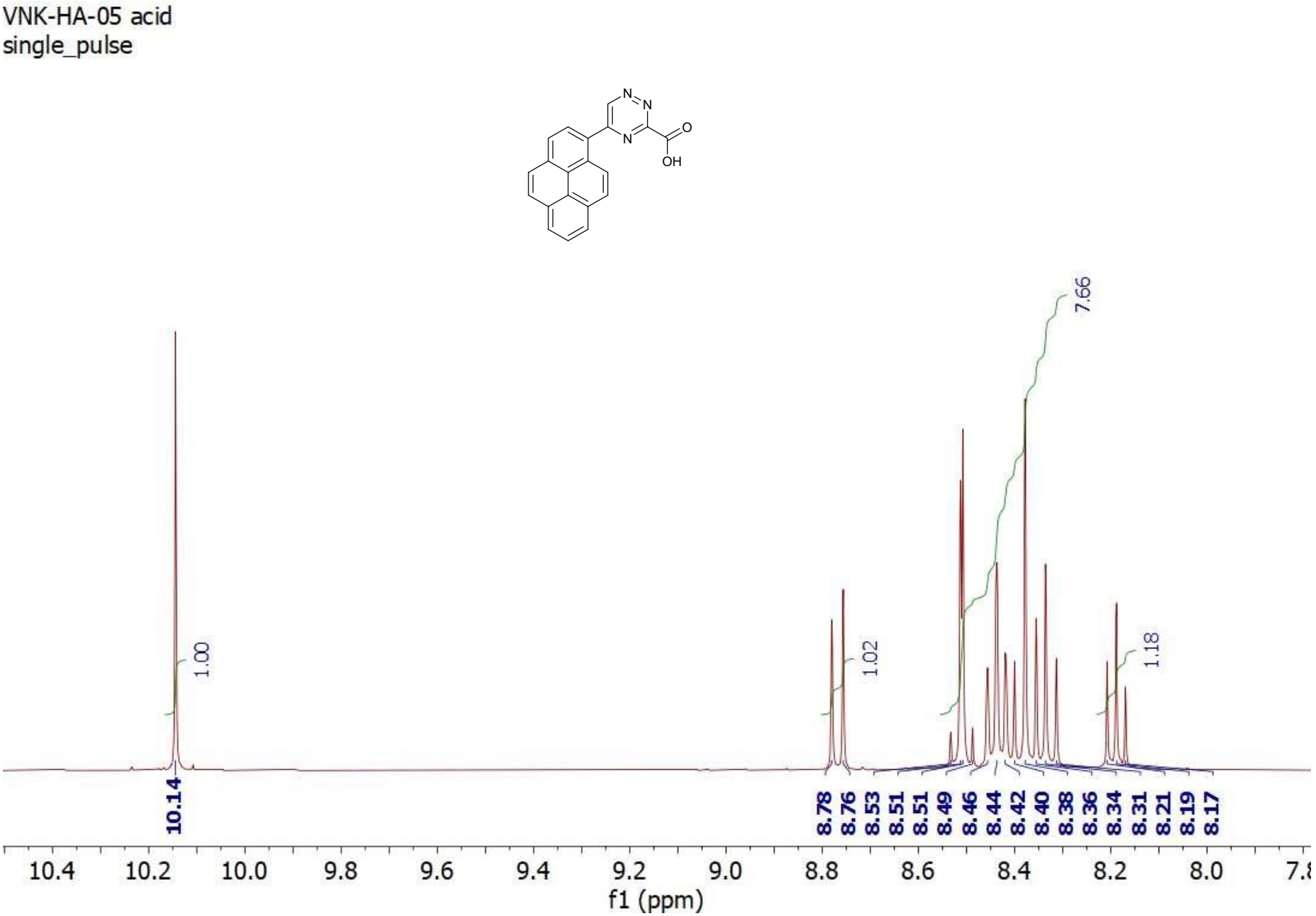


Figure S6. An aromatic region of ^{1}H NMR spectrum of **VNK-HA-05 acid** in DMSO-D_6.

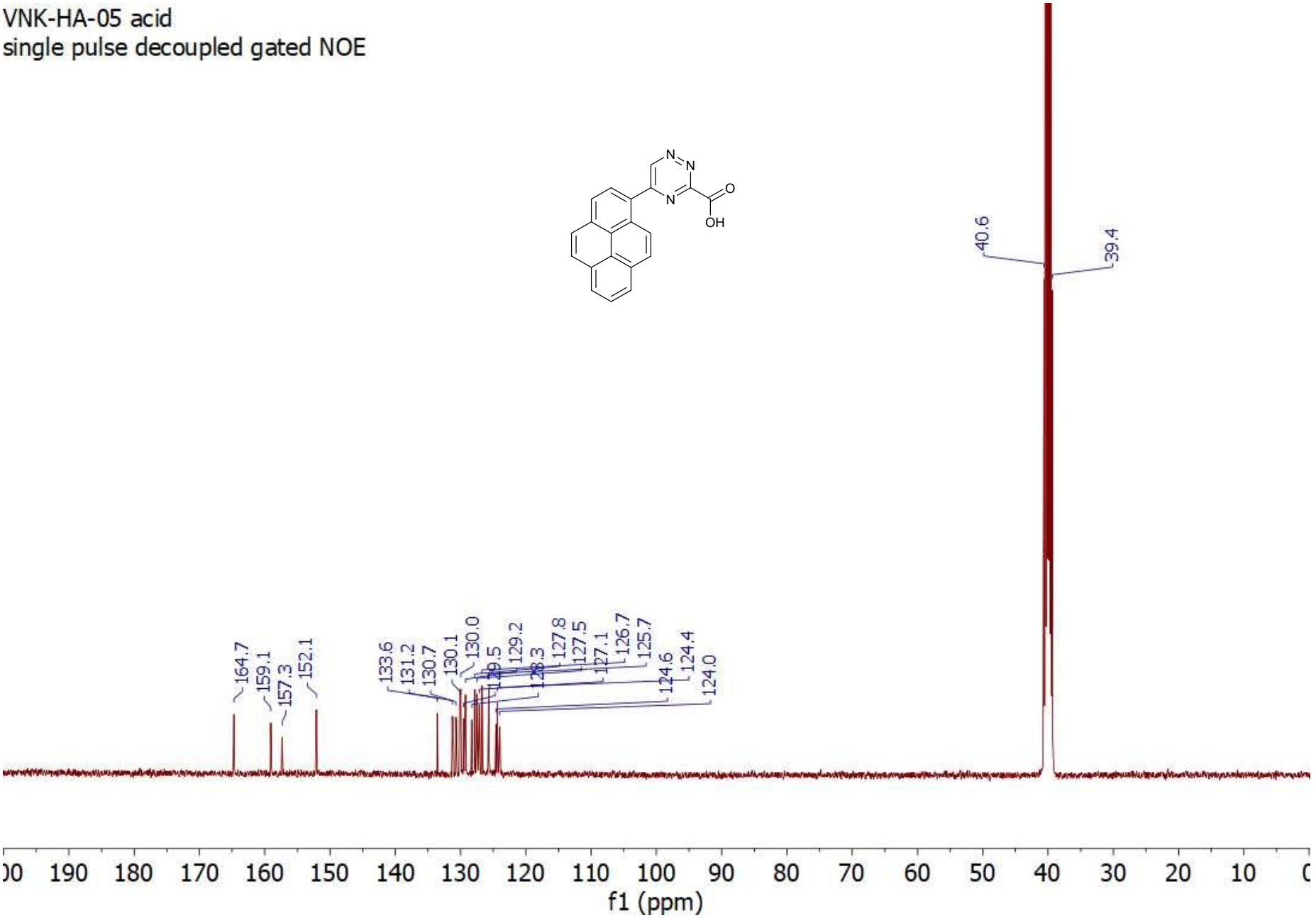


Figure S7. ^{13}C NMR spectrum of **VNK-HA-05 acid** in DMSO-D_6

VNK-HA-05 acid
single pulse decoupled gated NOE

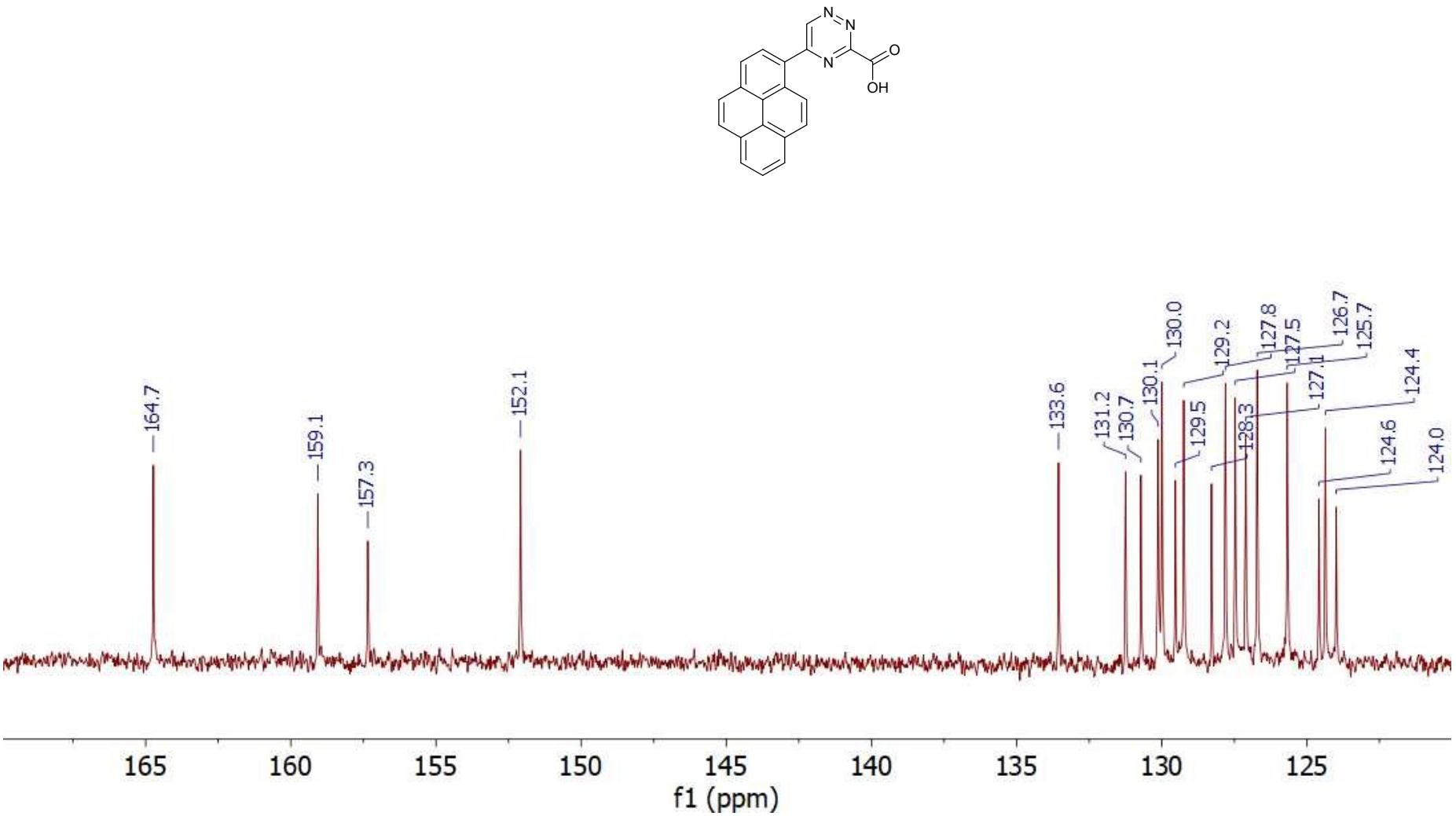


Figure S8. An aromatic region of ^{13}C NMR spectrum of **VNK-HA-05 acid** in DMSO-D_6

VNK-HA-11
single_pulse

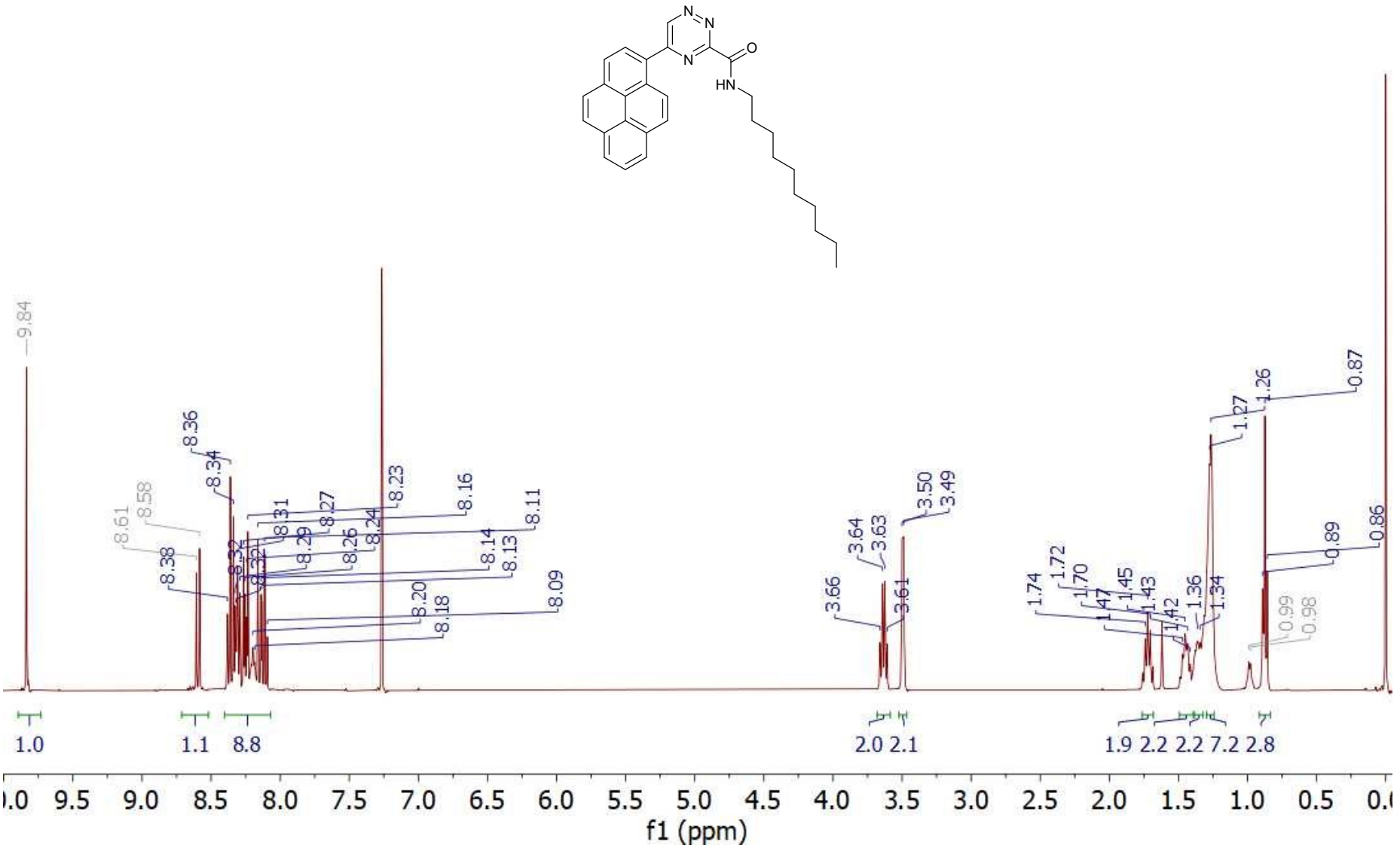


Figure S9. A ^{1}H NMR spectrum of **VNK-HA-11** in $CDCl_3$

VNK-HA-11
single_pulse

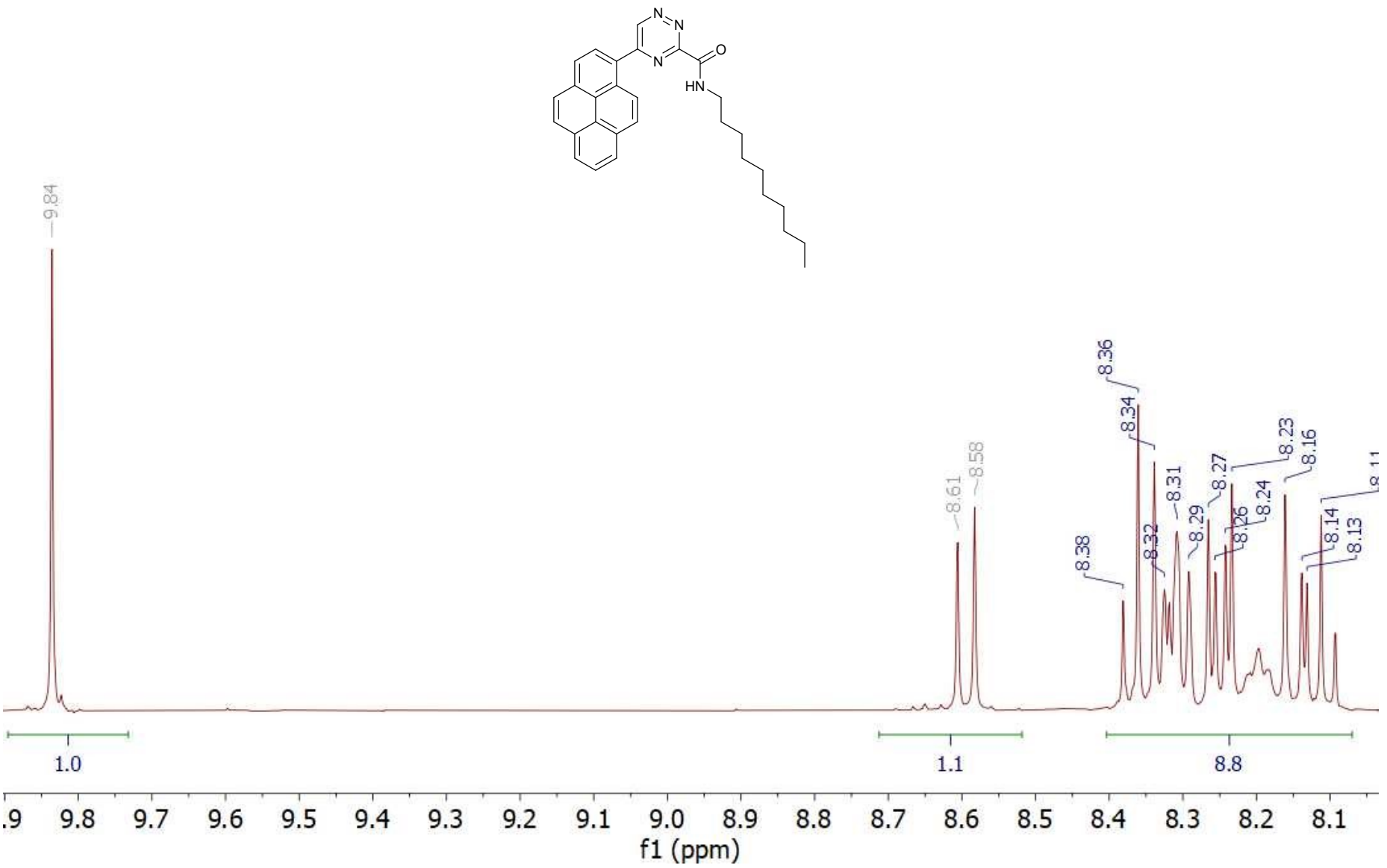


Figure S10. An aromatic region of ^{1}H NMR spectrum of **VNK-HA-11** in $CDCl_3$

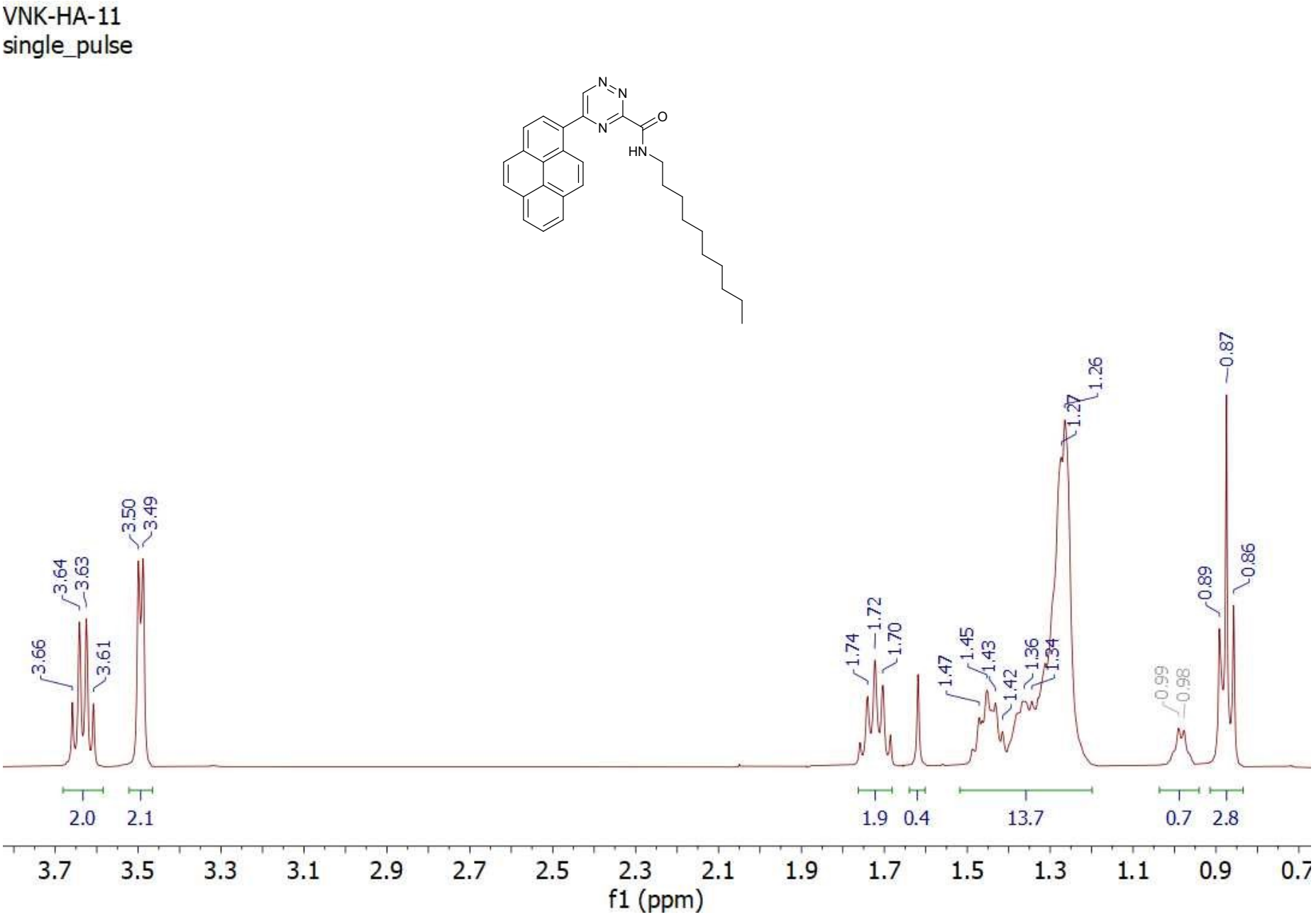


Figure S11. An aliphatic region of ^{1}H NMR spectrum of **VNK-HA-11** in $CDCl_3$

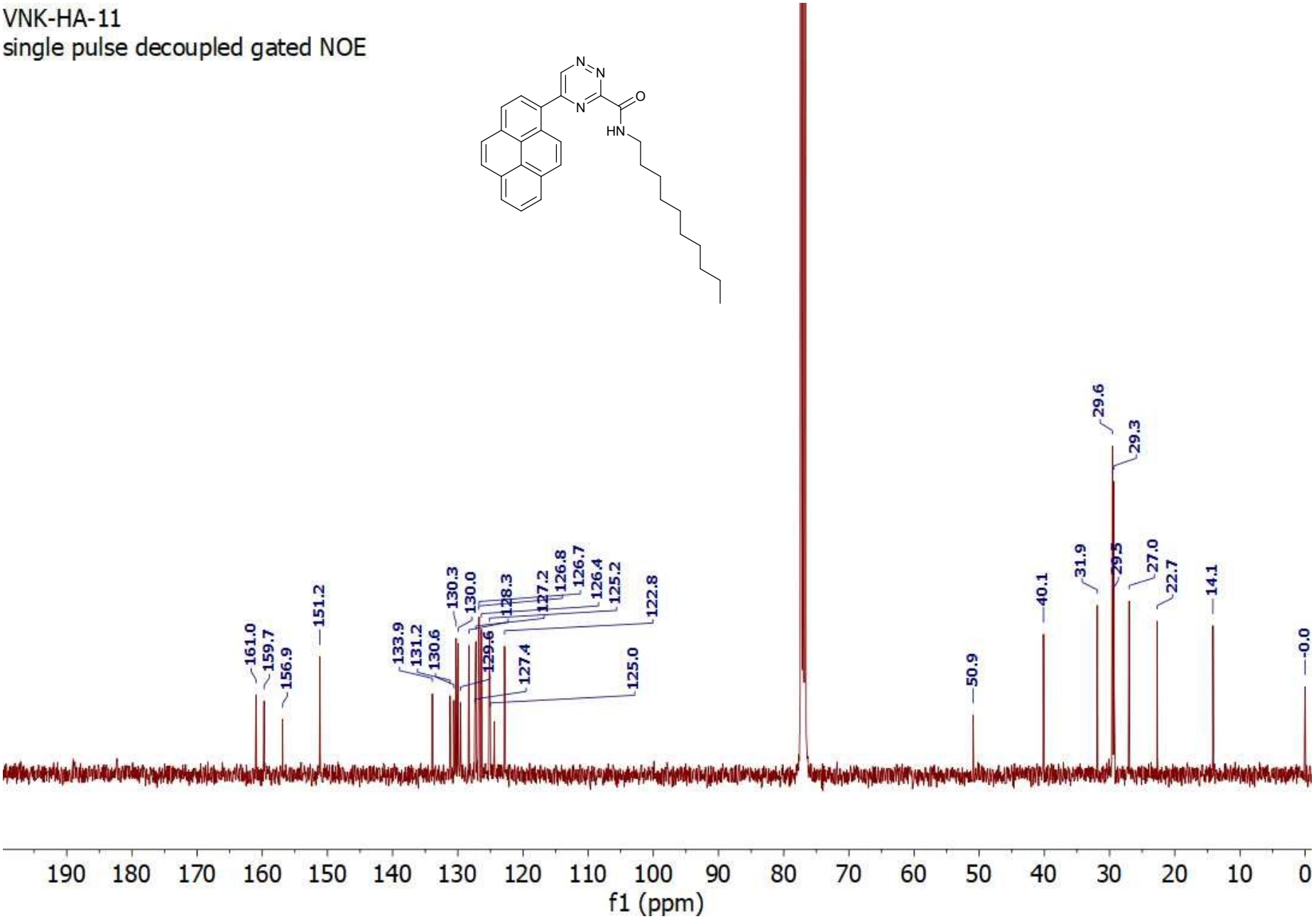


Figure S12. ^{13}C NMR spectrum of **VNK-HA-11** in $CDCl_3$

VNK-HA-11
single pulse decoupled gated NOE

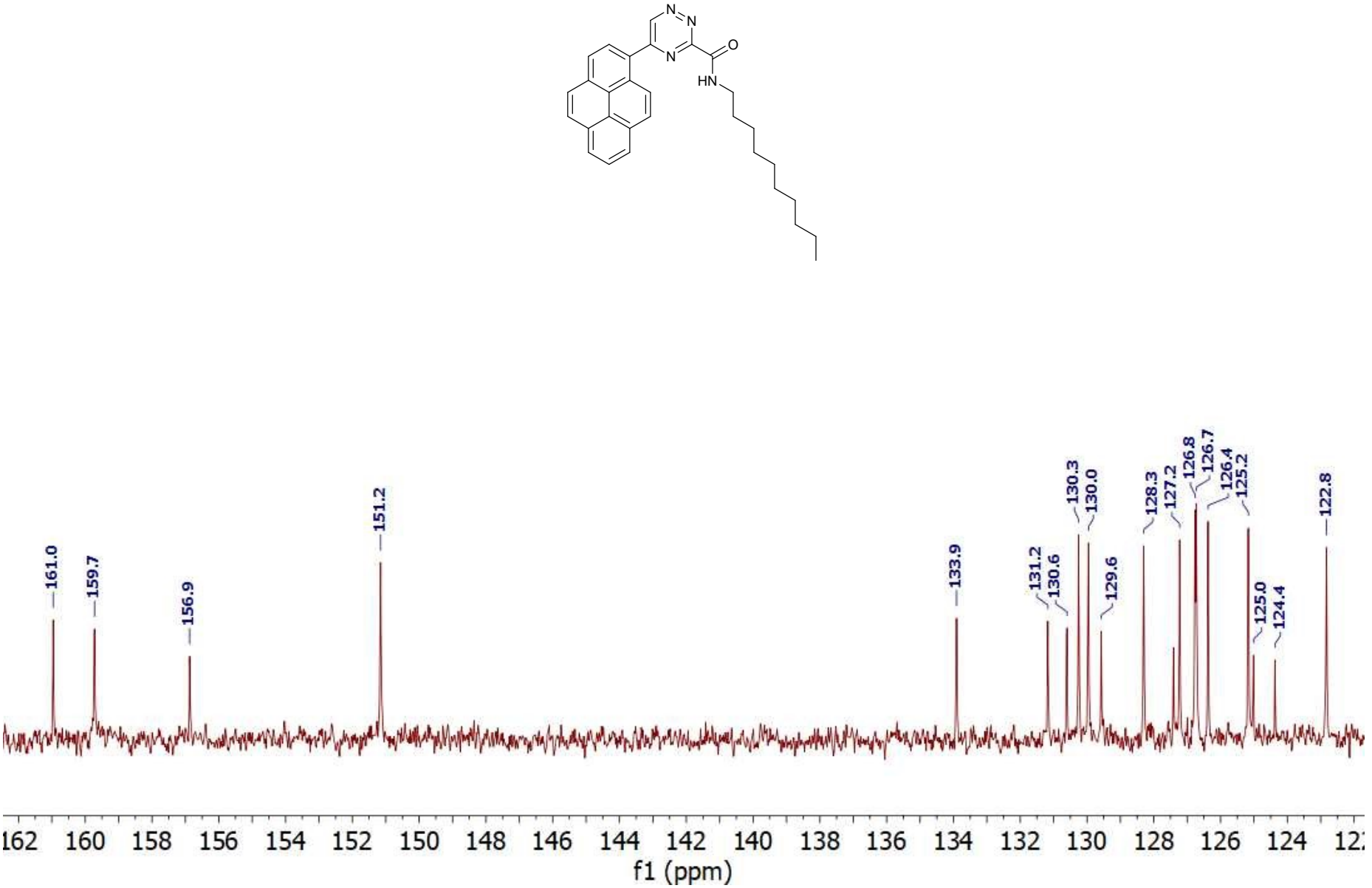


Figure S13. An aromatic region of ^{13}C NMR spectrum of **VNK-HA-11** in $CDCl_3$

VNK-HA-11
single pulse decoupled gated NOE

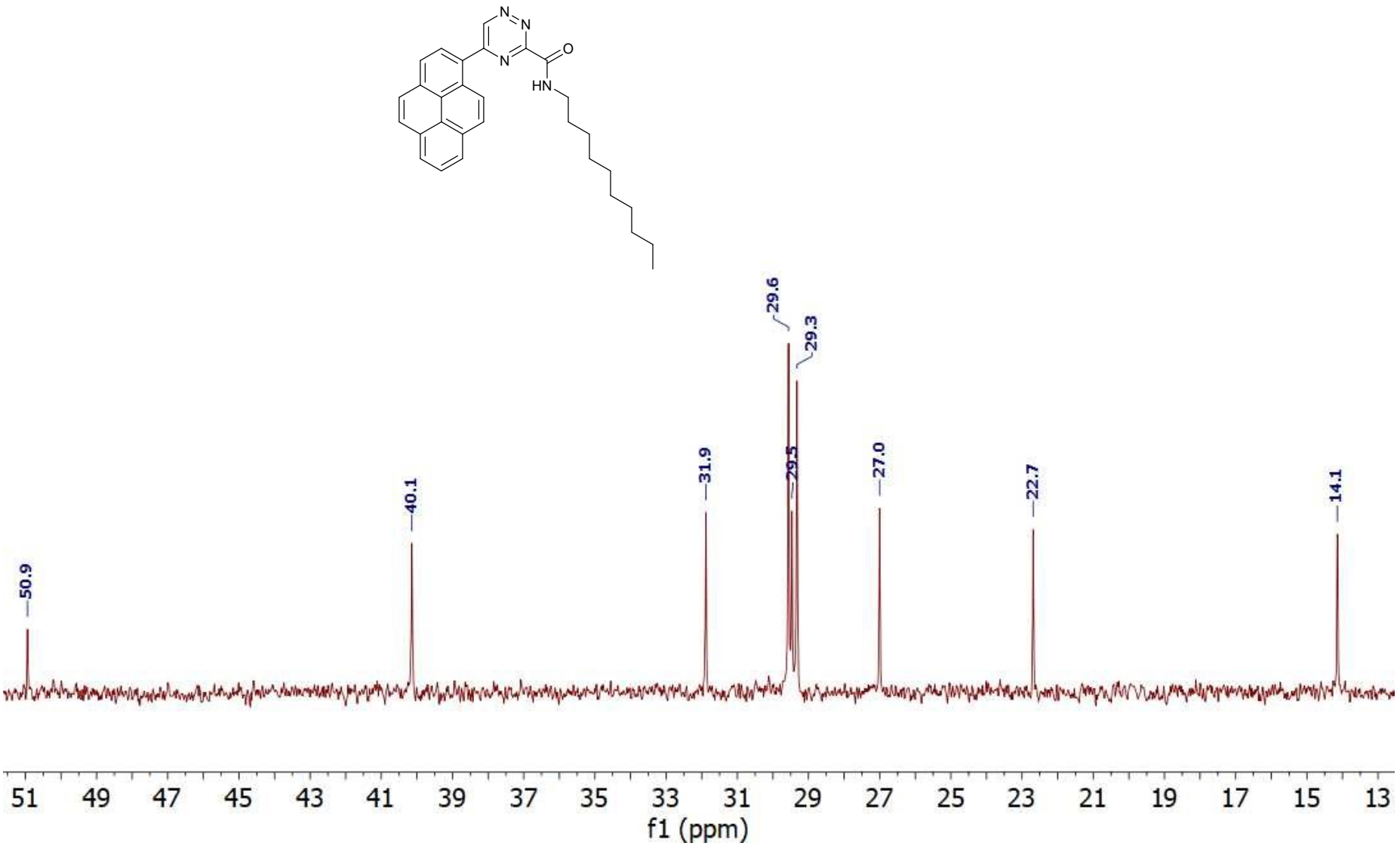


Figure S14. An aliphatic region of ^{13}C NMR spectrum of **VNK-HA-11** in $CDCl_3$ (signal at 50.9 is a signal of residual methanol)

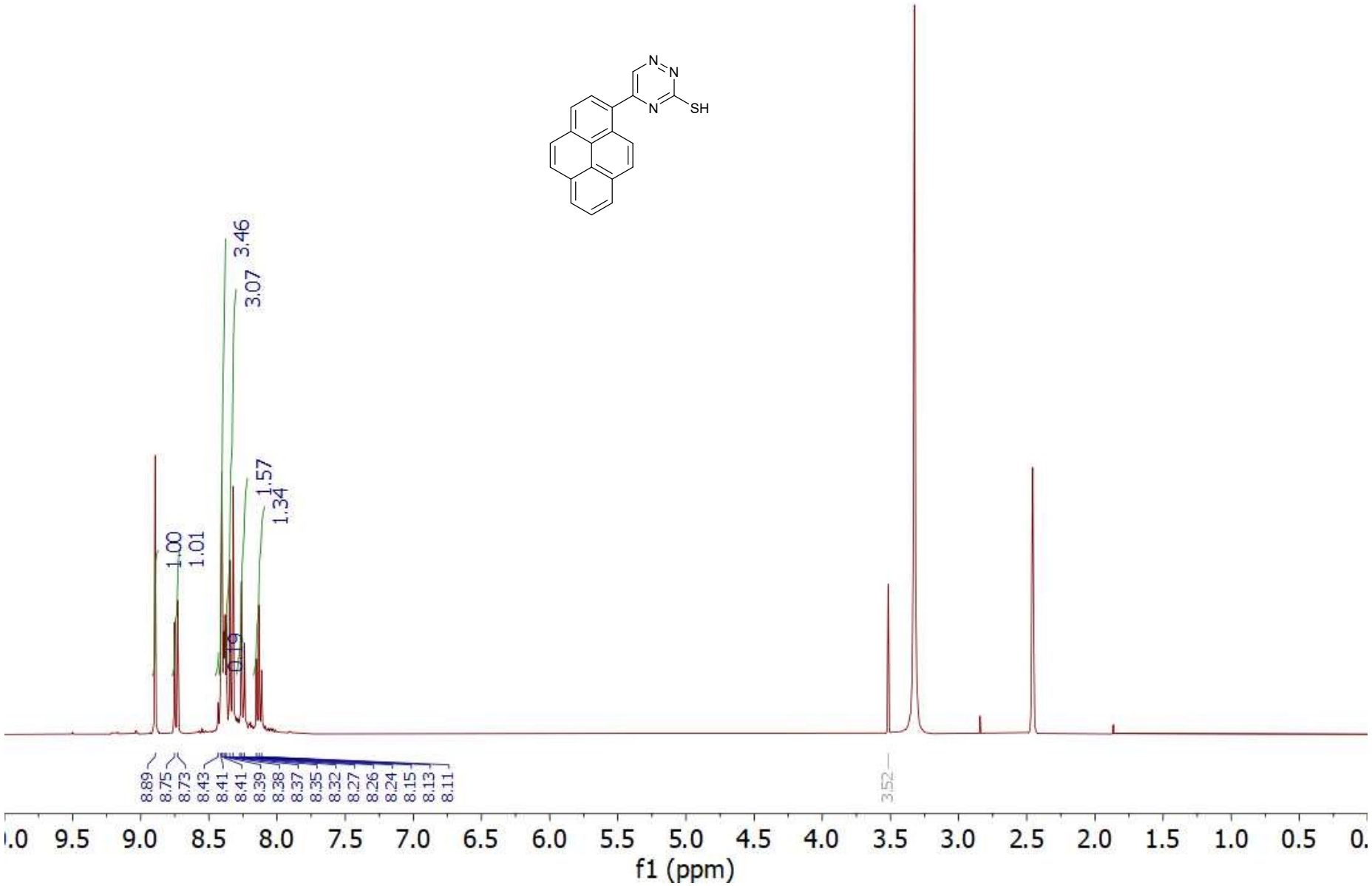


Figure S15. A ^{13}C NMR spectrum of **VNK-JMP-03** in DMSO-D_6

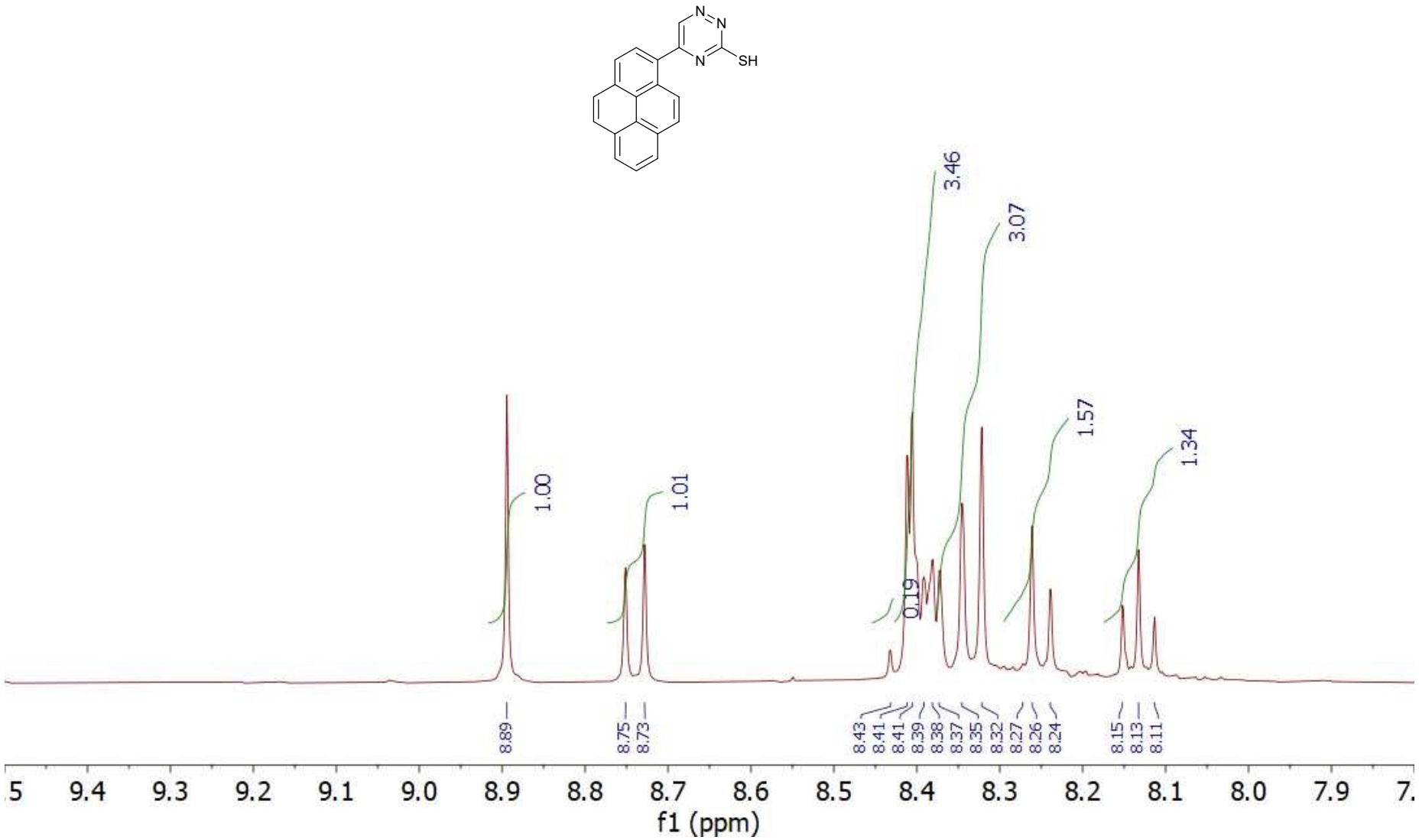


Figure S16. An aromatic region of ^{1}H NMR spectrum of **VNK-JMP-03** in DMSO-D_6

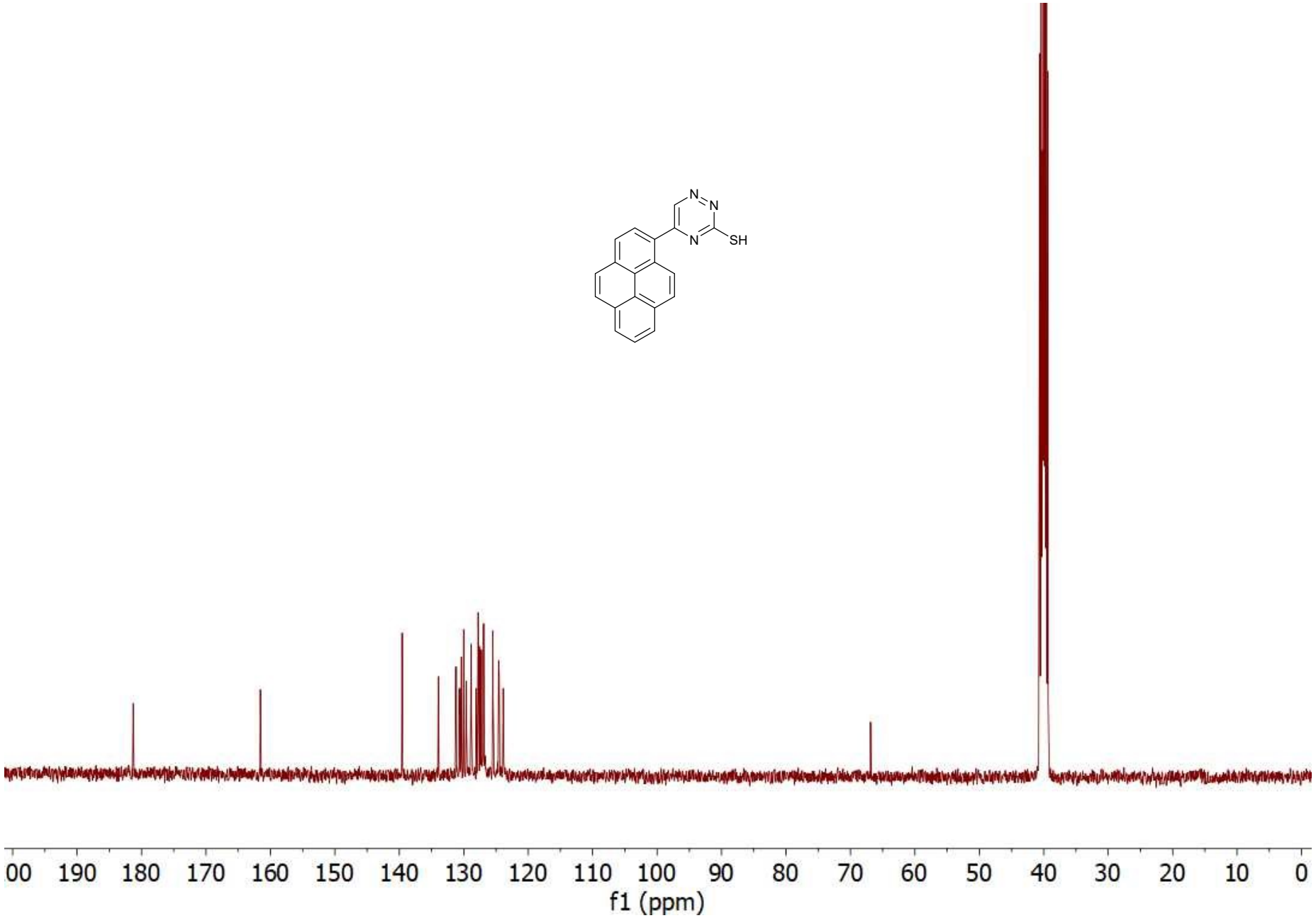


Figure S17. A ^{13}C NMR spectrum of **VNK-JMP-03** in DMSO-D_6

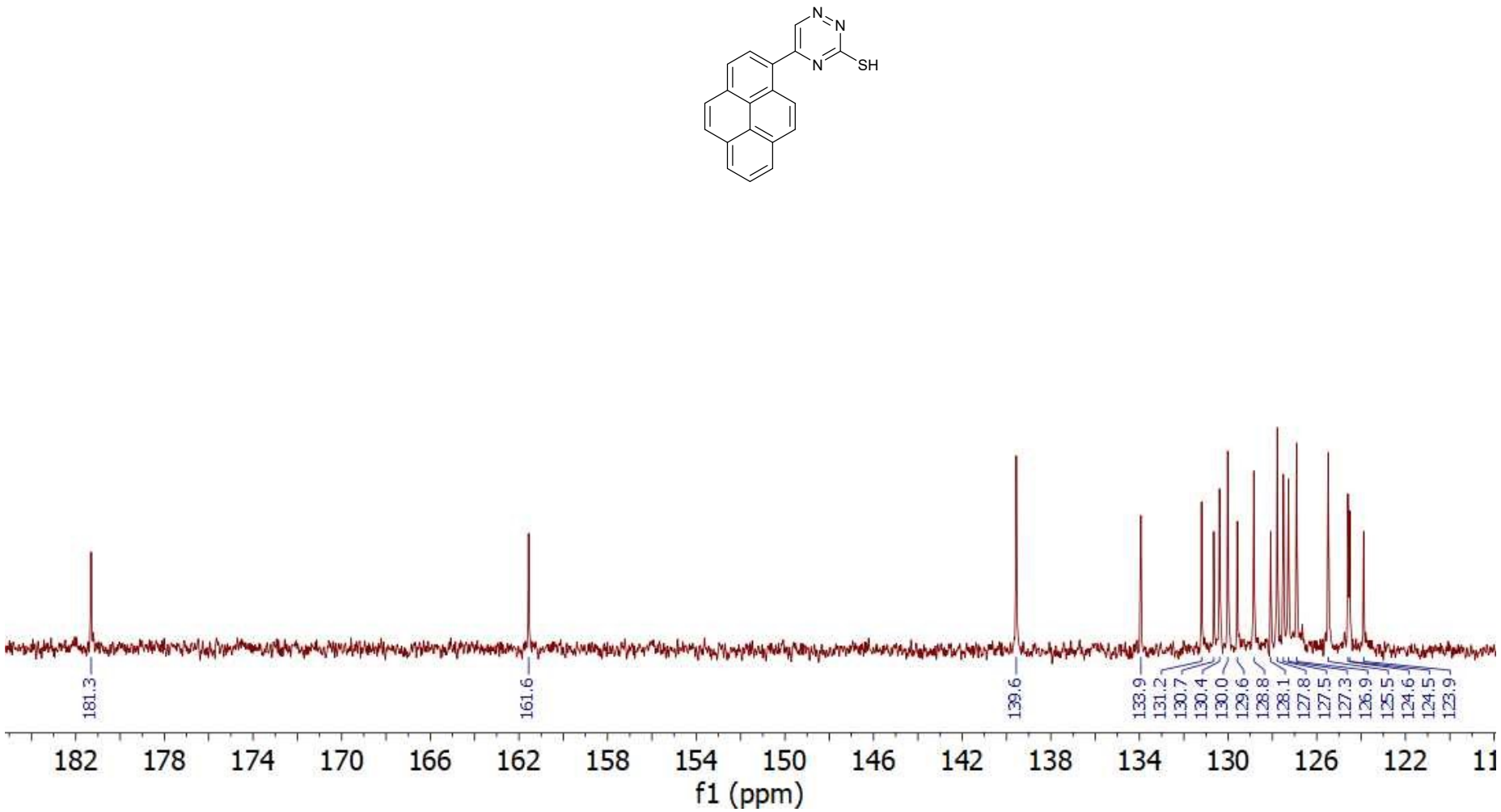


Figure S18. An aromatic region of ^{13}C NMR spectrum of **VNK-JMP-03** in DMSO-D_6

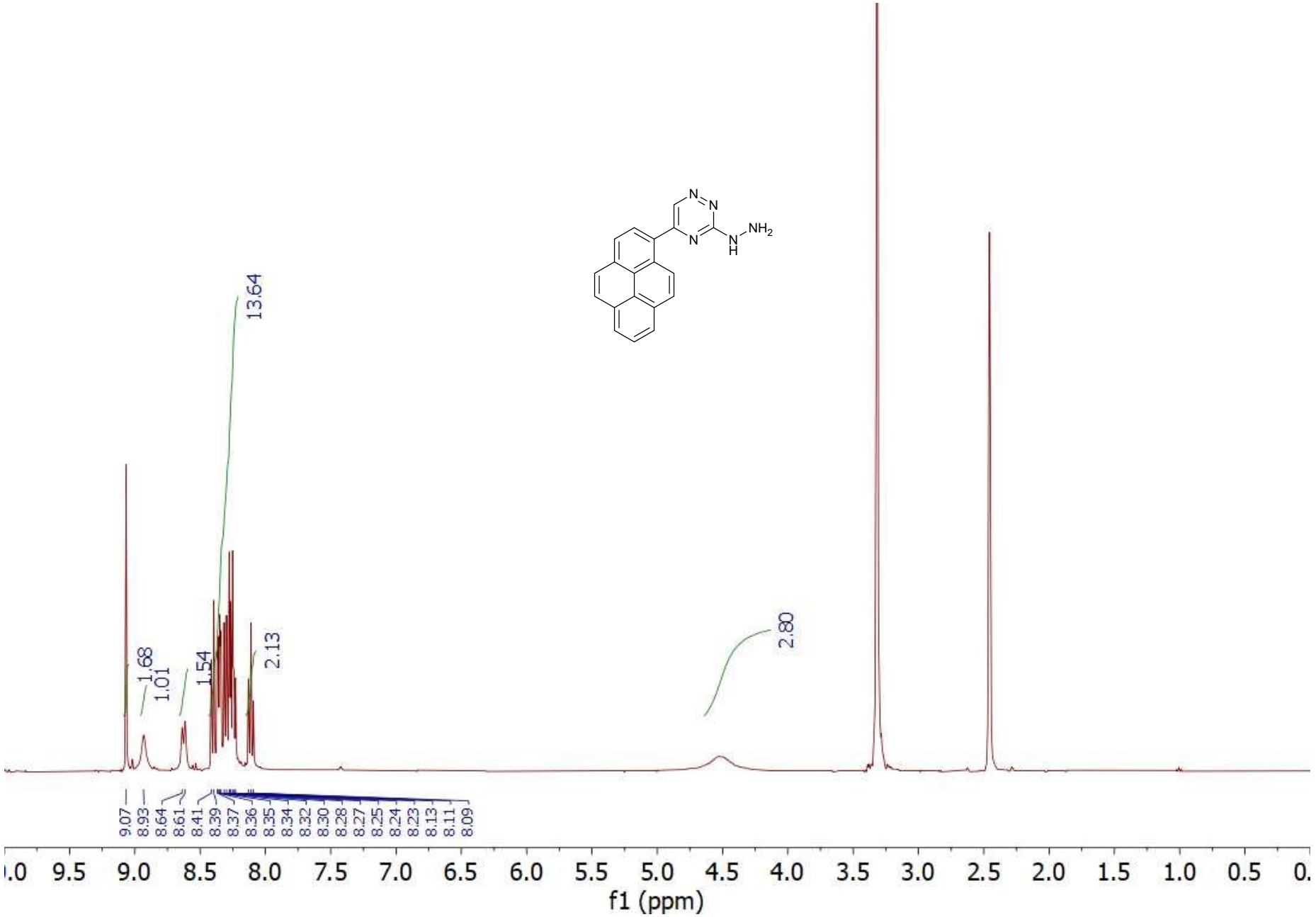


Figure S19. A ^{1}H NMR spectrum of **VNK-JMP-04** in DMSO-D_6

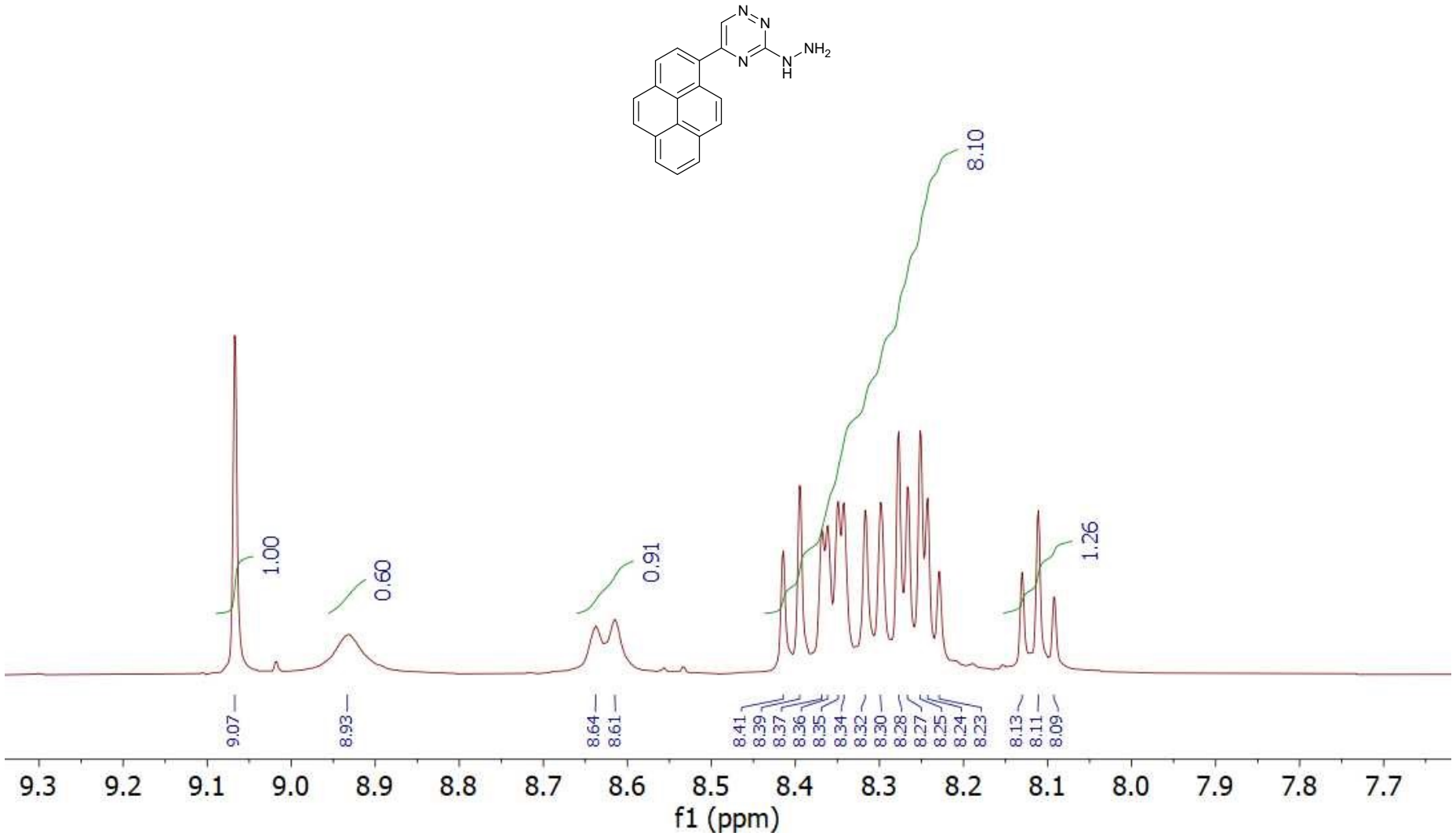


Figure S20. An aromatic region of ^{1}HNMR spectrum of **VNK-JMP-04** in DMSO-D_6

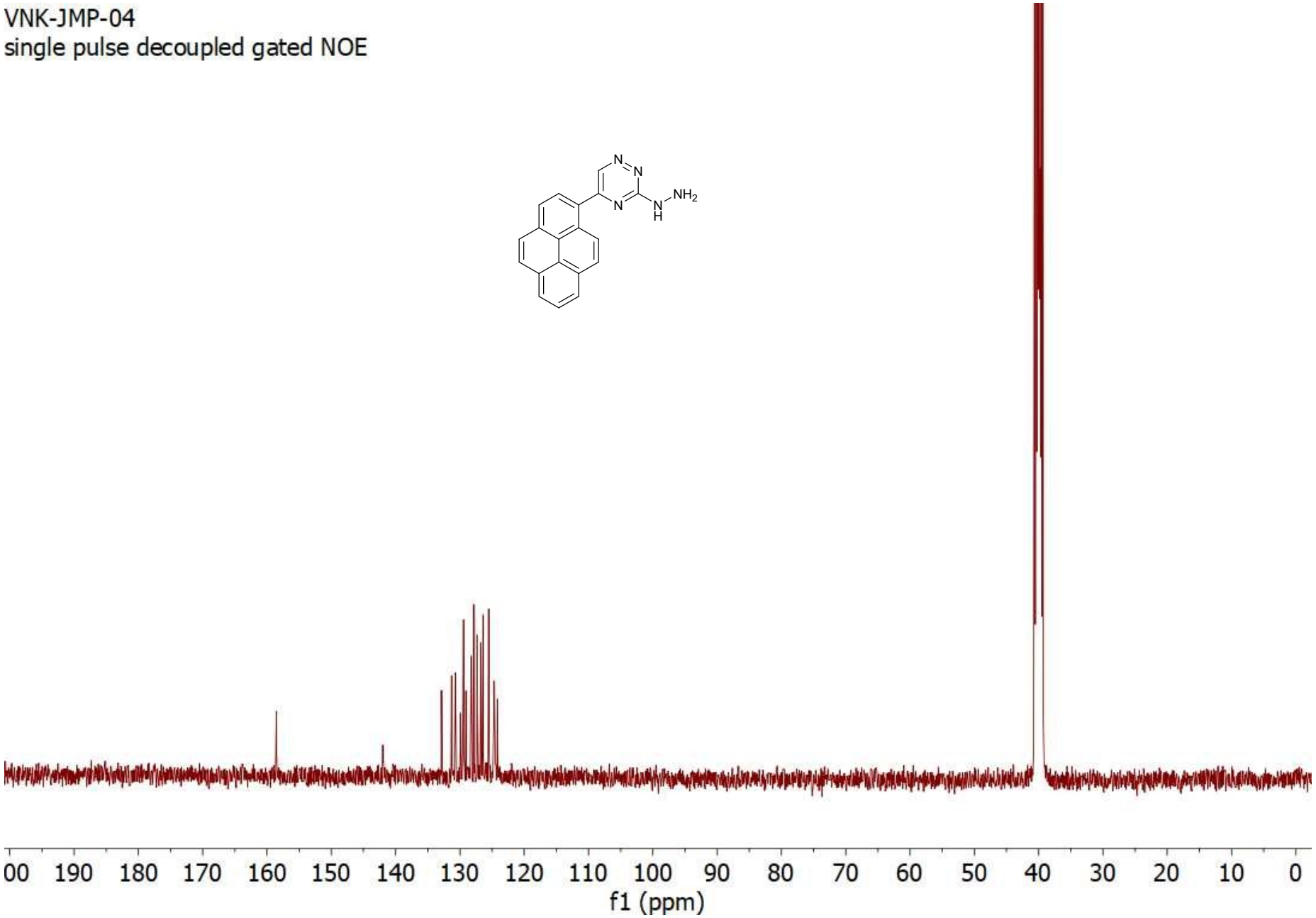


Figure S21. A ^{13}C NMR spectrum of **VNK-JMP-04** in DMSO-D_6

VNK-JMP-04
single pulse decoupled gated NOE

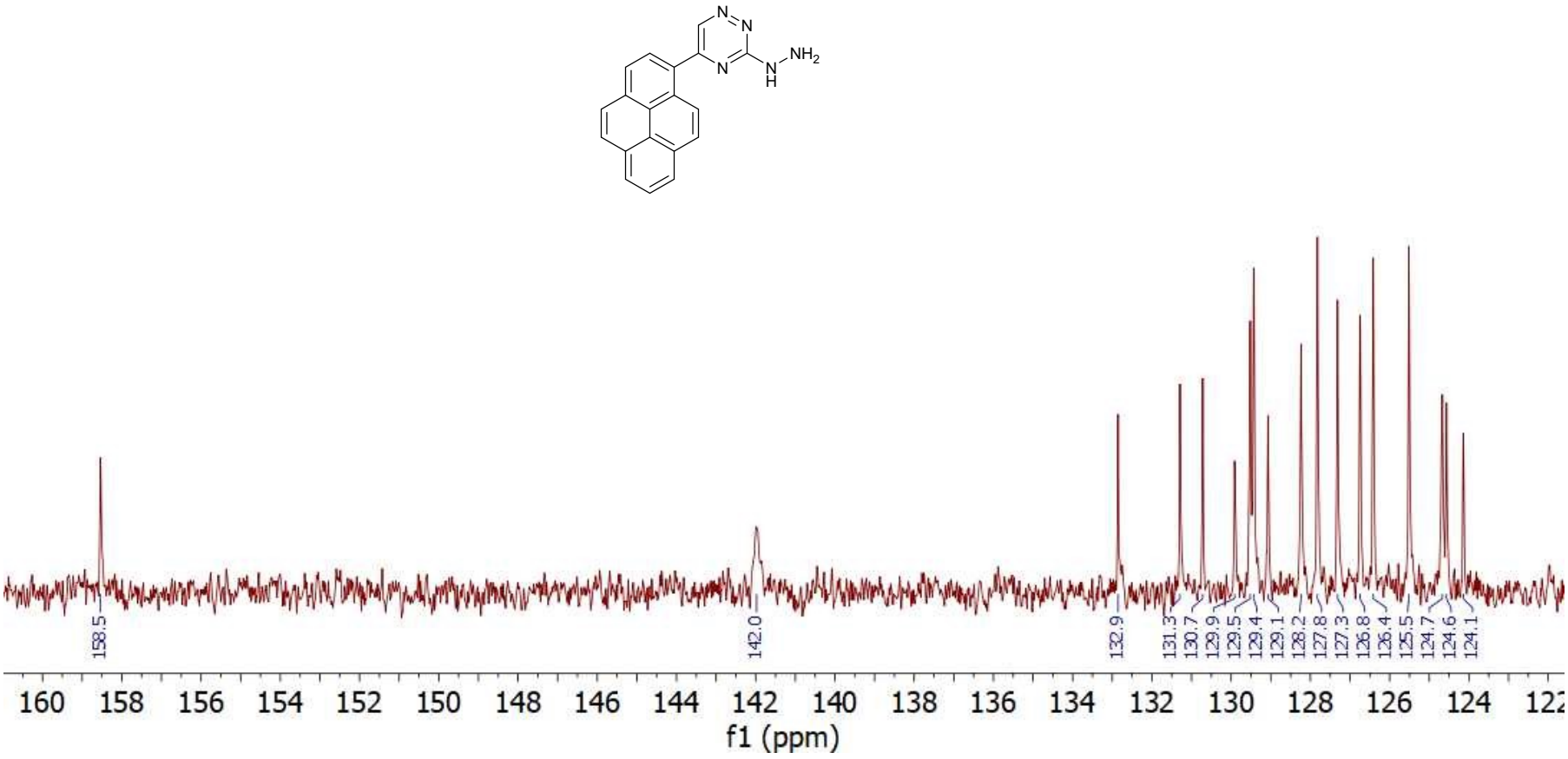


Figure S22. An aromatic region of ^{13}C NMR spectrum of **VNK-JMP-04** in DMSO-D_6

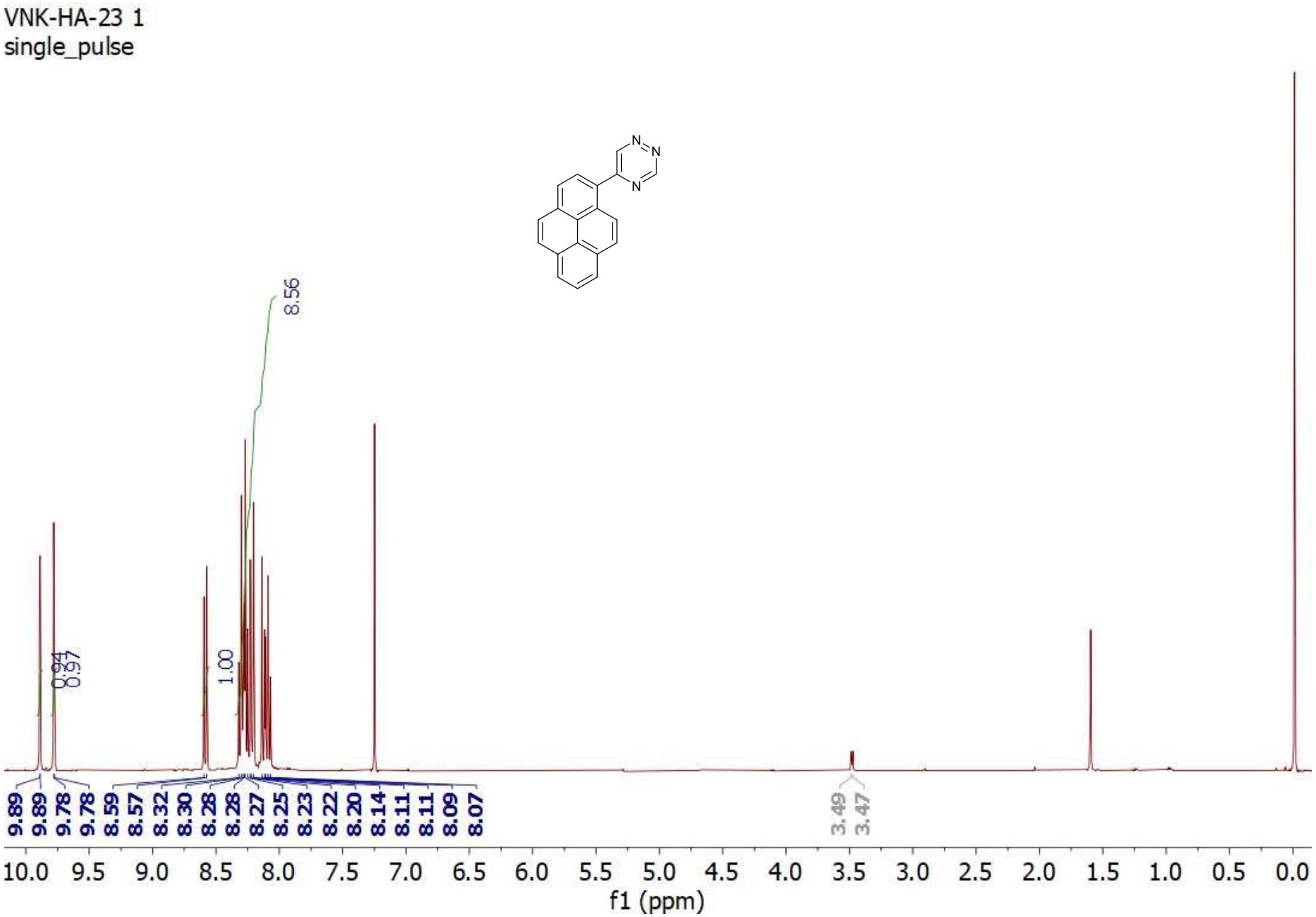


Figure S23. A ^{1}H NMR spectrum of **VNK-HA-23** in $CDCl_3$

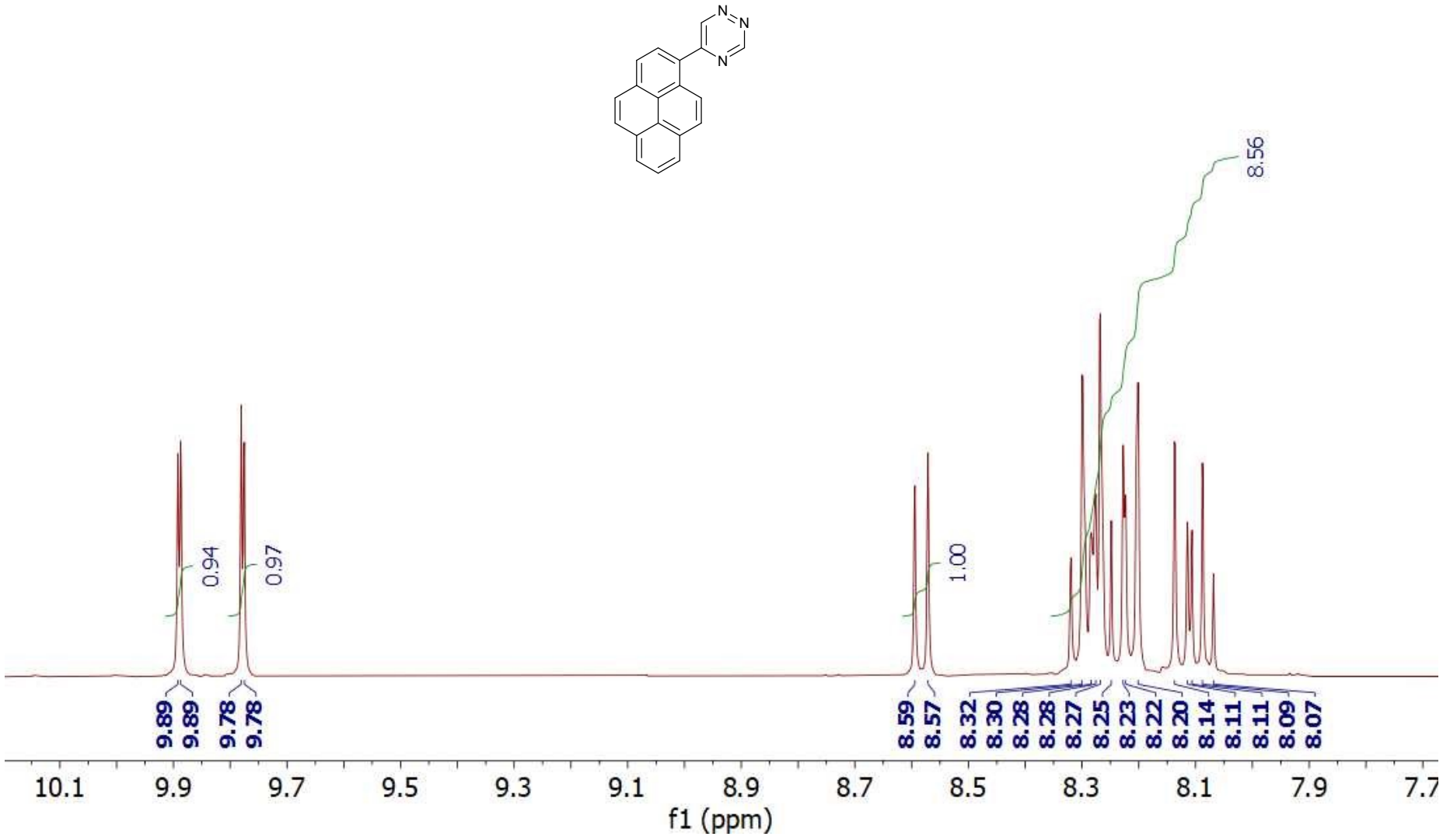


Figure S24. An aromatic region of ^{1}H NMR spectrum of **VNK-HA-23** in $CDCl_3$

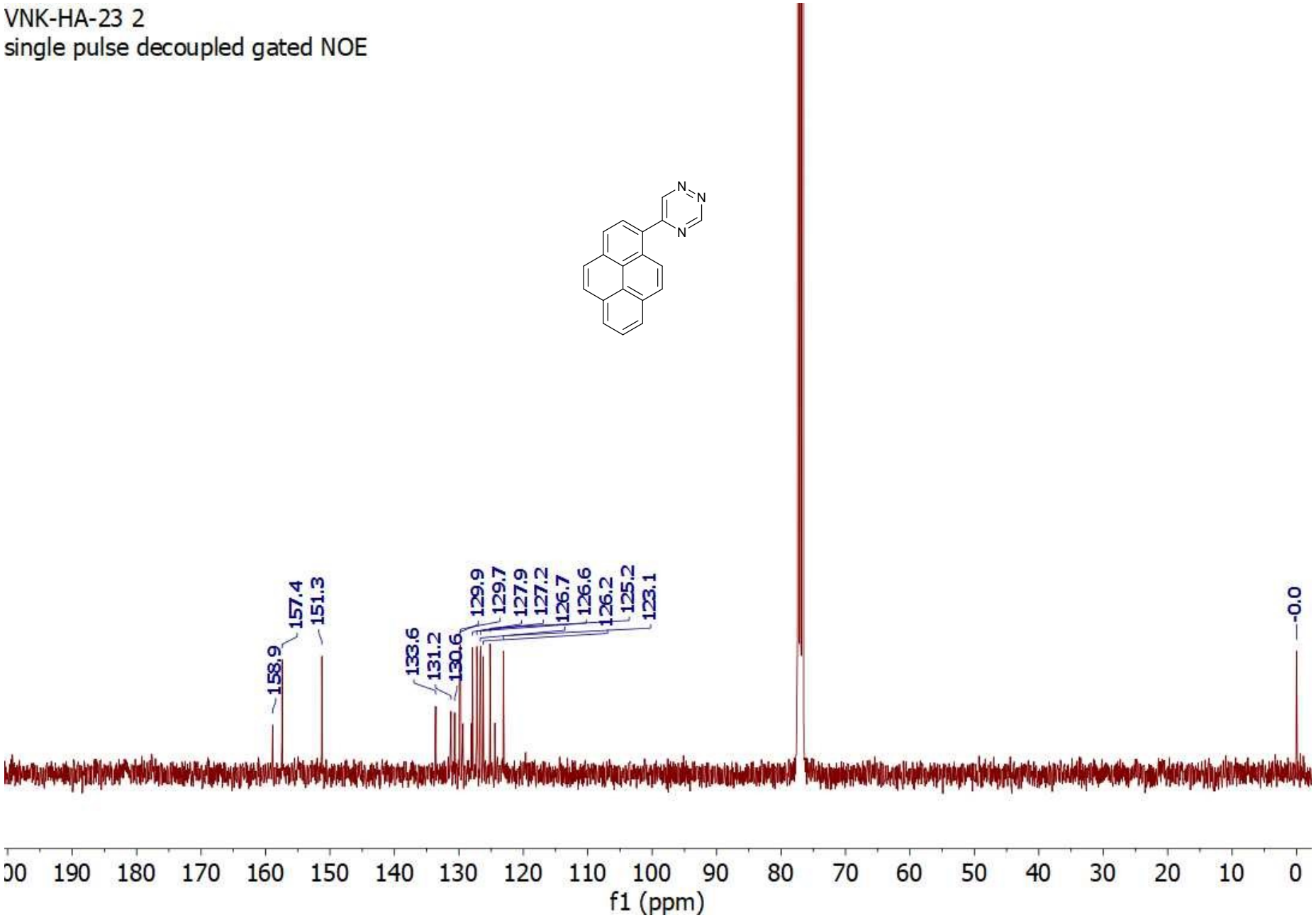


Figure S25. A ^{13}C NMR spectrum of **VNK-HA-23** in $CDCl_3$

VNK-HA-23 2
single pulse decoupled gated NOE

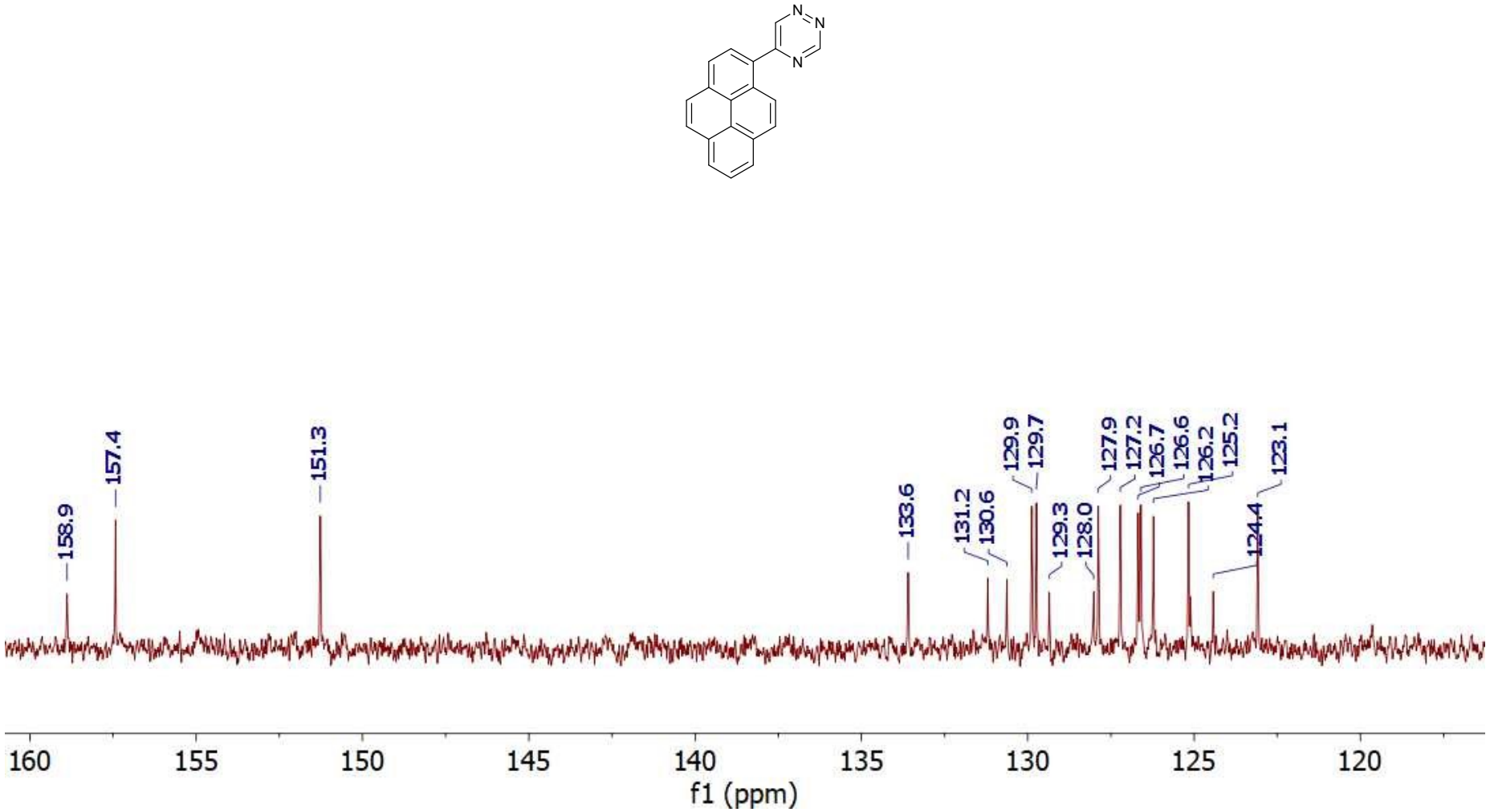


Figure S26. An aromatic region of ^{13}C NMR spectrum of **VNK-HA-23** in $CDCl_3$

Kinetics measurements

(a) Reaction of compounds **5**, **6**, **7** and **10** with s-TCO derivative **12**

The reaction between the triazine substrates (Compounds **5**, **6**, **7** and **10**) and s-TCO were carried out in DMSO at 25°C under pseudo-first order conditions, with s-TCO in at least 10-fold excess. Reactions were followed by monitoring the loss of the substrate absorbance spectrophotometrically at a suitable wavelength. Observed pseudo-first-order rate constants, k_{obs}, were obtained using nonlinear regression of the monoexponential loss of absorbance with time. Second order rate constants, k_2, were obtained from linear regression of plots of k_{obs} against s-TCO concentration. Second order plots are shown in Figures S27 to S30.

Stock solutions of the substrate and BCN (both 2 mM) were prepared in DMSO and diluted as necessary. The reactions were carried out at 25˚C using Pharmacia Ultrospec 2000 UV-visible spectrophotometer. Suitable wavelengths at which to carry out the reaction kinetics were determined using a similar procedure to that outlined above but measuring sequential wavelength scans (200 to 600 nm) to determine the wavelength at which the maximum absorbance change took place during the reaction.

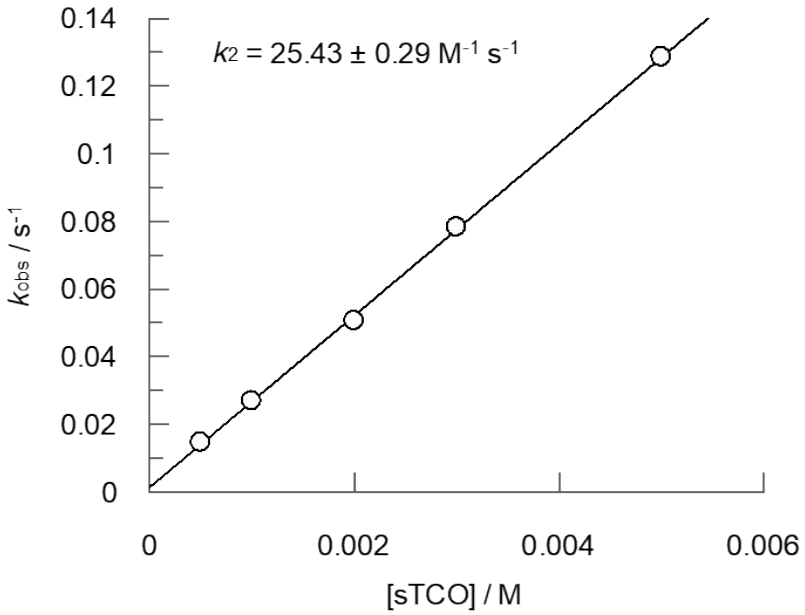


Figure S27: Plot of observed pseudo-first-order rate constant, k_{obs}, against sTCO concentration for the reaction with compound **5**. The slope, which is equal to the second order rate constant, k_2, is shown on the plot. The reactions were carried out in DMSO at 25°C under pseudo-first-order conditions, with [Compound **5**]$_0$ = 0.5 x 10^{-4} M and sTCO concentrations as stated on the x-axis. Pseudo-first-order rate constants, k_{obs}, were obtained from measuring the monoexponential decay in absorbance at 410nm using non-linear least squares analysis.

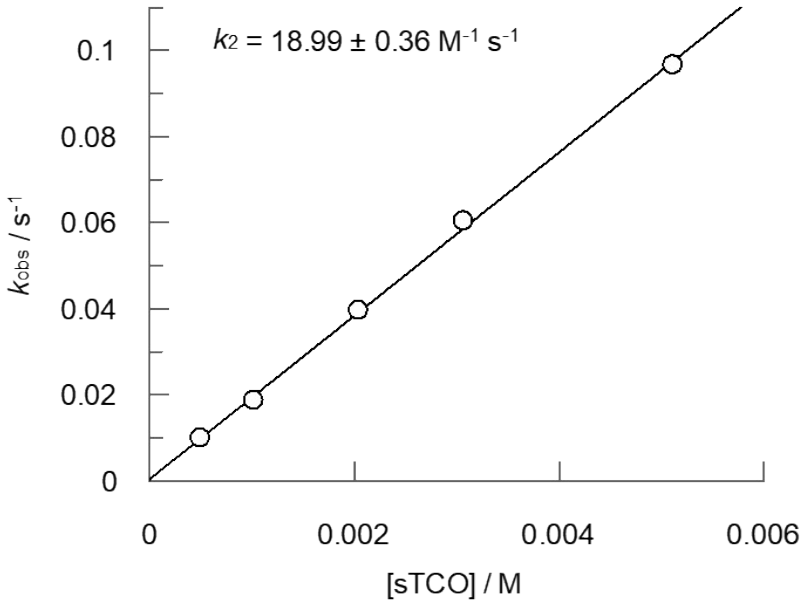


Figure S28: Plot of observed pseudo-first-order rate constant, k_{obs}, against sTCO concentration for the reaction with compound 6. The slope, which is equal to the second order rate constant, k_2, is shown on the plot. The reactions were carried out in DMSO at 25°C under pseudo-first-order conditions, with [Compound **6**]$_0$ = 1.0 x 10^{-4} M and sTCO concentrations as stated on the x-axis. Pseudo-first-order rate constants, k_{obs}, were obtained from measuring the monoexponential decay in absorbance at 420nm using non-linear least squares analysis.

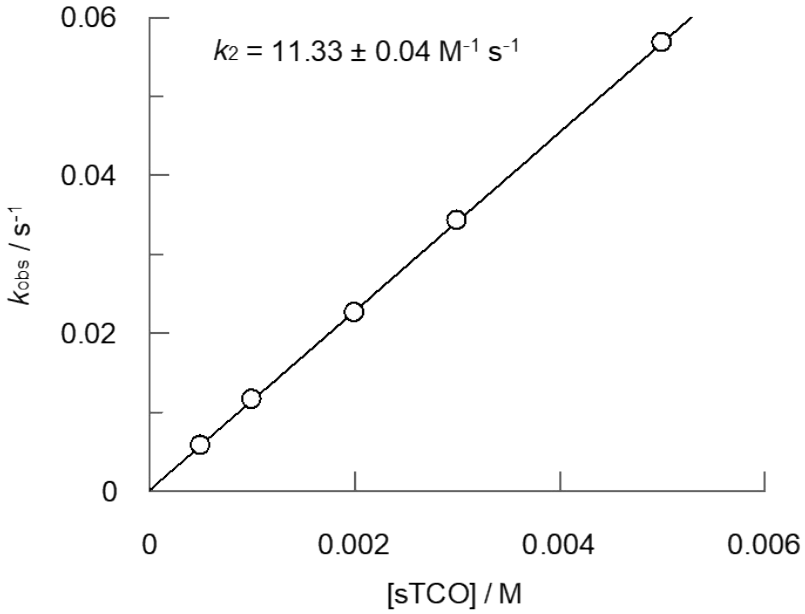


Figure S29: Plot of observed pseudo-first-order rate constant, k_{obs}, against sTCO concentration for the reaction with compound **7**. The slope, which is equal to the second order rate constant, k_2, is shown on the plot. The reactions were carried out in DMSO at 25°C under pseudo-first-order conditions, with [Compound **7**]$_0$ = 0.5 x 10^{-4} M and sTCO concentrations as stated on the x-axis. Pseudo-first-order rate constants, k_{obs}, were obtained from measuring the monoexponential decay in absorbance at 420nm using non-linear least squares analysis.

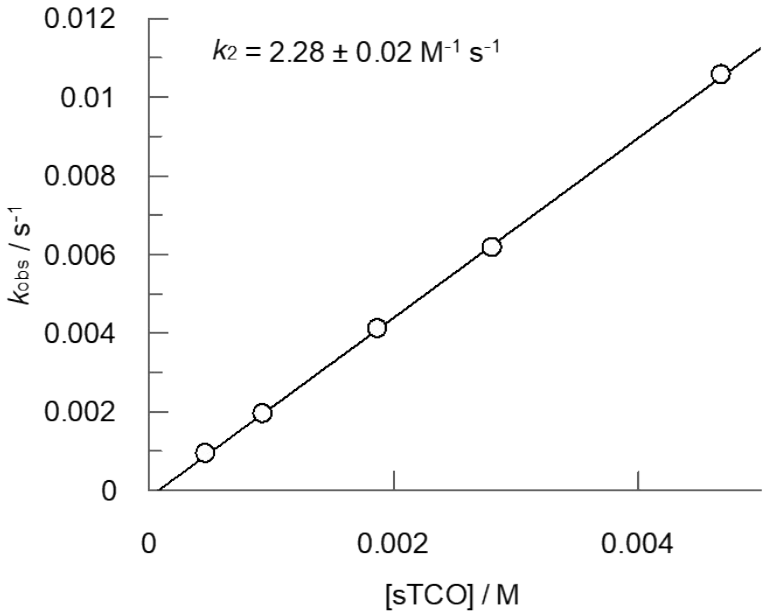


Figure S30: Plot of observed pseudo-first-order rate constant, k_{obs}, against sTCO concentration for the reaction with compound **10**. The slope, which is equal to the second order rate constant, k_2, is shown on the plot. The reactions were carried out in DMSO at 25°C under pseudo-first-order conditions, with [Compound **10**]$_0$ = 0.5 x 10^{-4} M and sTCO concentrations as stated on the x-axis. Pseudo-first-order rate constants, k_{obs}, were obtained from measuring the monoexponential decay in absorbance at 400nm using non-linear least squares analysis.

(b) Reaction of compounds **5**, **6**, **7** and **10** with TCO derivative **11**

The reaction between the triazine substrates and TCO derivative **11** were carried out in DMSO at 25°C under pseudo-first order conditions, with TCO in at least 10-fold excess. Reactions were followed by monitoring the loss of the substrate absorbance spectrophotometrically at a suitable wavelength. Observed pseudo-first-order rate constants, k_{obs}, were obtained using nonlinear regression of the monoexponential loss of absorbance with time. Second order rate constants, k_2, were obtained from linear regression of plots of k_{obs} against TCO concentration. Second order plots are shown in Figures S31 to S34.

Stock solutions of the substrates and BCN (both 2 mM) were prepared in DMSO and diluted as necessary. The reactions were carried out at 25˚C using a Pharmacia Ultrospec 2000 UV-visible spectrophotometer. Suitable wavelengths at which to carry out the reaction kinetics were determined using a similar procedure to that outlined above but measuring sequential wavelength scans (200 to 600 nm) to determine the wavelength at which the maximum absorbance change took place during the reaction.

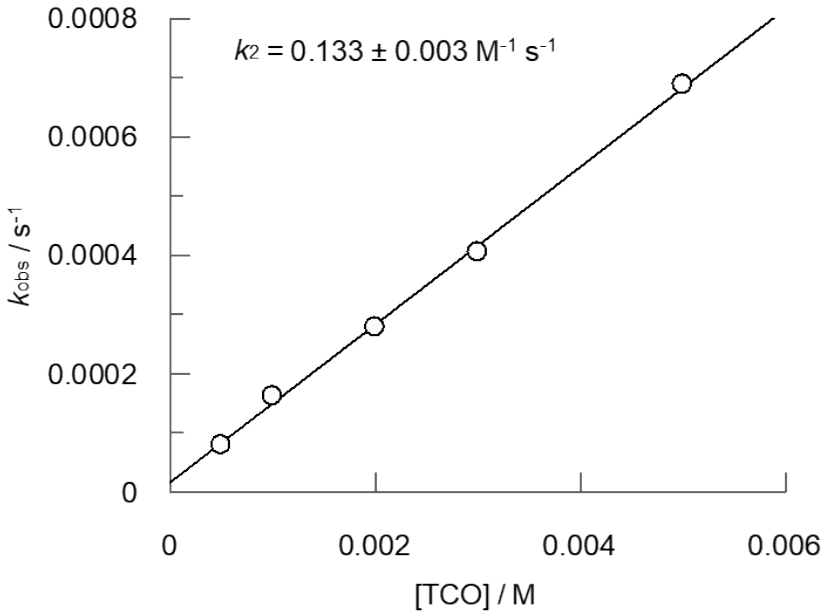


Figure S31: Plot of observed pseudo-first-order rate constant, k_{obs}, against TCO concentration for the reaction with compound **5**. The slope, which is equal to the second order rate constant, k_2, is shown on the plot. The reactions were carried out in DMSO at 25°C under pseudo-first-order conditions, with [Compound **5**]$_0$ = 0.5 x 10^{-4} M and TCO concentrations as stated on the x-axis. Pseudo-first-order rate constants, k_{obs}, were obtained from measuring the monoexponential decay in absorbance at 410nm using non-linear least squares analysis.

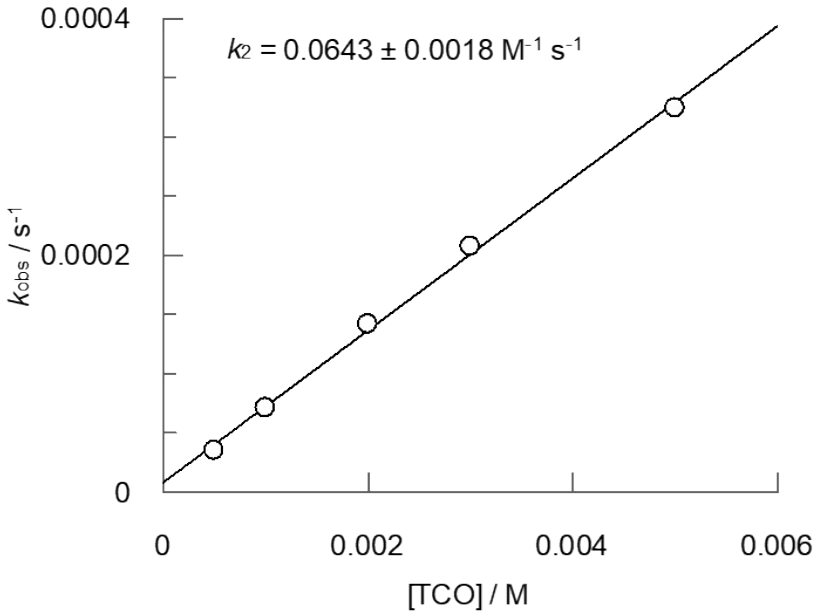


Figure S32: Plot of observed pseudo-first-order rate constant, k_{obs}, against TCO derivative concentration for the reaction with compound **6**. The slope, which is equal to the second order rate constant, k_2, is shown on the plot. The reactions were carried out in DMSO at 25°C under pseudo-first-order conditions, with [Compound **6**]$_0$ = 0.5 x 10^{-4} M and TCO concentrations as stated on the x-axis. Pseudo-first-order rate constants, k_{obs}, were obtained from measuring the monoexponential decay in absorbance at 420nm using non-linear least squares analysis.

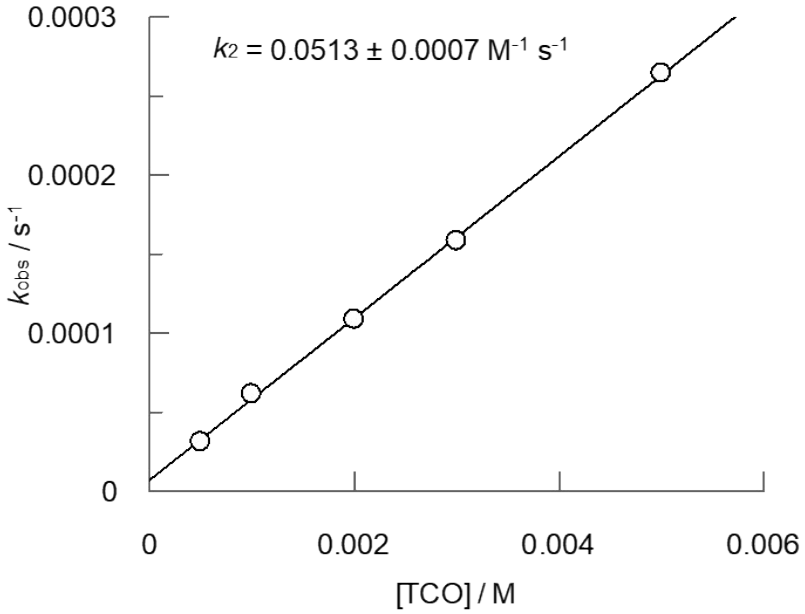


Figure S33: Plot of observed pseudo-first-order rate constant, k_{obs}, against TCO concentration for the reaction with compound **7**. The slope, which is equal to the second order rate constant, k_2, is shown on the plot. The reactions were carried out in DMSO at 25°C under pseudo-first-order conditions, with [Compound **7**]$_0$ = 0.5 x 10^{-4} M and TCO derivative **11** concentrations as stated on the x-axis. Pseudo-first-order rate constants, k_{obs}, were obtained from measuring the monoexponential decay in absorbance at 420nm using non-linear least squares analysis.

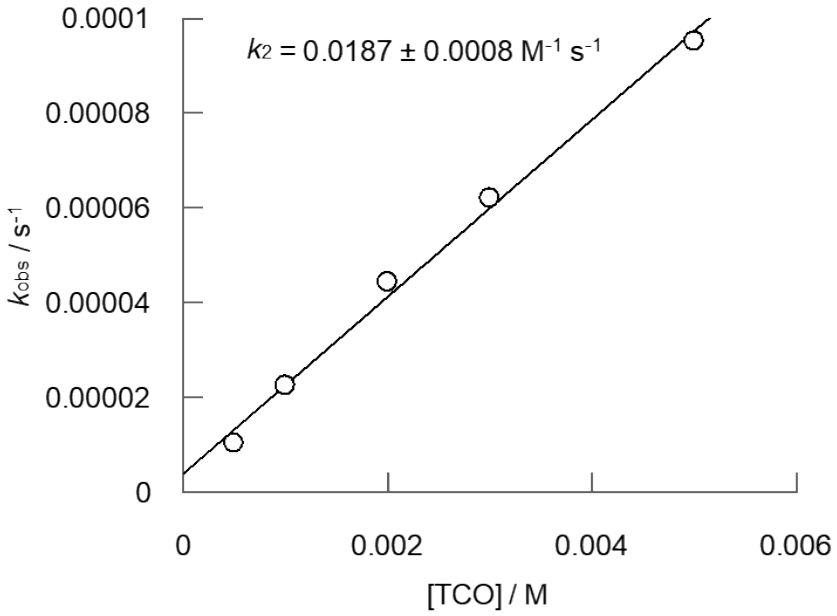


Figure S34: Plot of observed pseudo-first-order rate constant, k_{obs}, against sTCO concentration for the reaction with compound **10**. The slope, which is equal to the second order rate constant, k_2, is shown on the plot. The reactions were carried out in DMSO at 25°C under pseudo-first-order conditions, with [Compound **10**]$_0$ = 0.5 x 10^{-4} M and TCO derivative **11** concentrations as stated on the x-axis. Pseudo-first-order rate constants, k_{obs}, were obtained from measuring the monoexponential decay in absorbance at 400nm using non-linear least squares analysis.

(c) Reaction of compounds **5**, **6** and **10** with BCN derivative **10**

Second-order rate constants (k_2) for the reactions of compounds **5**, **6**, and **10** with BCN derivative **13** in DMSO-d_6 were determined at 25 °C by mixing equimolar amounts of each substrate (**5**, **6**, or **10**) and BCN derivative **13** (0.5 mL each, 0.01 M final concentration) directly in an NMR tube. Reaction progress was monitored by following the disappearance of proton resonances on the triazine moiety of the substrate: for compounds 5 and 6, the H-6 proton resonance at δ 10.12 ppm; and for compound 10 and the loss of both H-6 and H-4 proton signals at ca. δ 10 ppm. 1,3,5-Trimethoxybenzene was included as an internal standard (0.01M). Second-order rate constants were obtained from plots of reciprocal concentration versus time (Figures S35 to S37). NMR processing and analysis was carried out in Mnova 16.0 (Mestrelab Research, S.L., Santiago de Compostela, Spain).

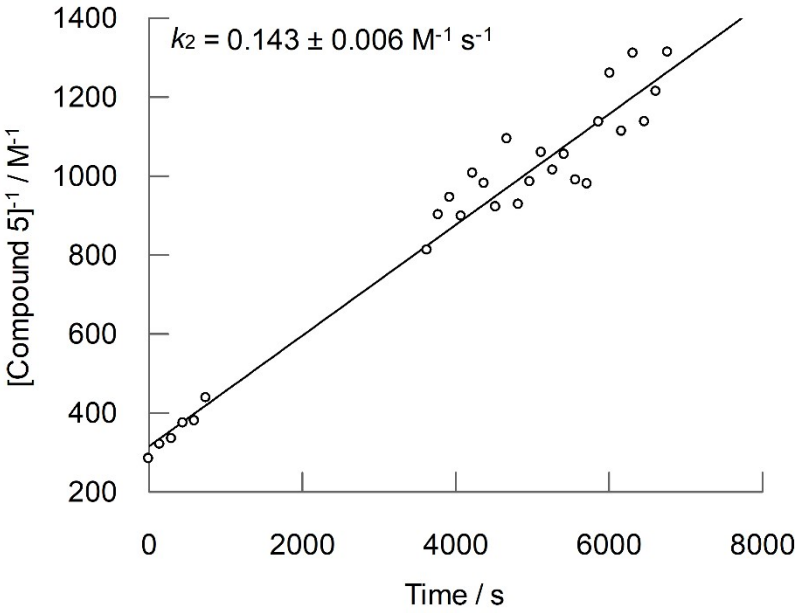


Figure S35 Second-order kinetic plot for the reaction of Compound **5** with BCN derivative **13** (0.01 M each) in DMSO-d_6 at 25 °C. Reaction progress was monitored by following the disappearance of the H-6 proton resonance on the triazine moiety of the substrate at δ 10.12 ppm. The slope of the fitted line corresponds to the second-order rate constant (k_2). 1,3,5-Trimethoxybenzene was included as an internal standard (0.01M). Data acquisition was interrupted between 900 and 3600 seconds.

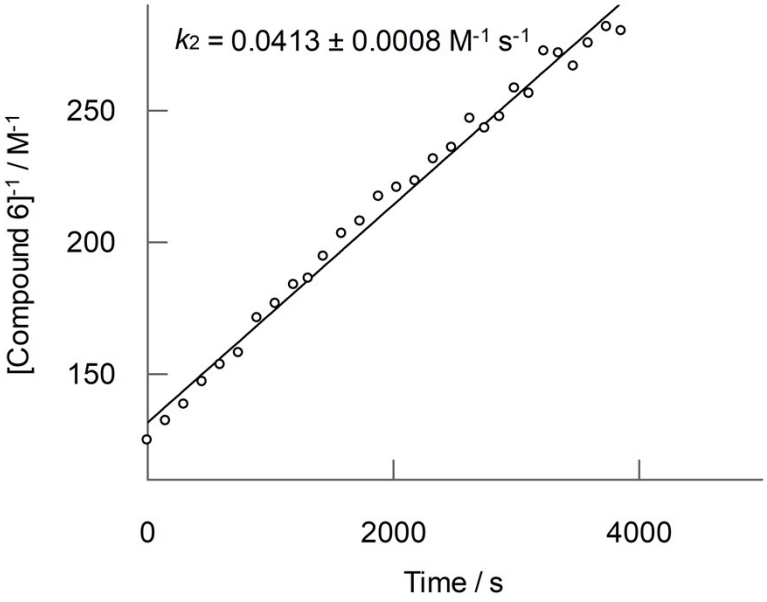


Figure S36 Second-order kinetic plot for the reaction of Compound **6** with BCN derivative **13** (0.01 M each) in DMSO-d_6 at 25 °C. Reaction progress was monitored by following the disappearance of the H-6 proton resonance on the triazine moiety of the substrate at δ 10.12 ppm. The slope of the fitted line corresponds to the second-order rate constant (k_2). 1,3,5-Trimethoxybenzene was included as an internal standard (0.01M).

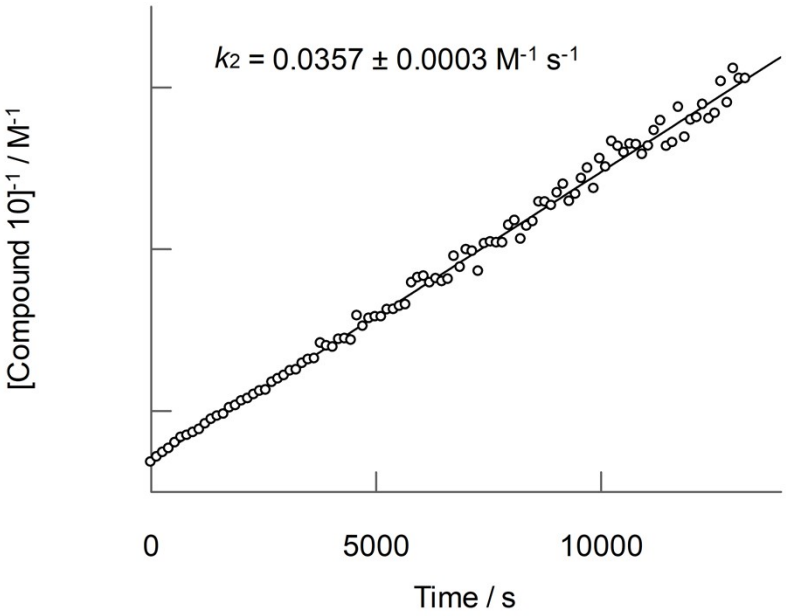


Figure S37 Second-order kinetic plot for the reaction of Compound **10** with BCN derivative **13** (0.01 M each) in DMSO-d_6 at 25 °C. Reaction progress was monitored by following the disappearance of the H-4 and H-6 proton resonances on the triazine moiety of the substrate at ca. δ 10 ppm. The slope of the fitted line corresponds to the second-order rate constant (k_2). 1,3,5-Trimethoxybenzene was included as an internal standard (0.01M).

Computational analysis

Coordinates of the lowest energy transition states determined for each reaction

5 bcn

C	-4.34968606041031	-1.30117944449814	-0.66732653939789
C	-5.21922317890975	-0.63242220214594	-1.53498880600259
C	-4.72494064551918	0.18516858281952	-2.54485466189948
C	-3.35488314881385	0.35283105683977	-2.70558886103850
C	-2.45338145458720	-0.29382512965293	-1.85330260564917
C	-2.94796008508087	-1.13177588637416	-0.82122811108865
C	-2.04055700939886	-1.77939447085389	0.07284200075178
C	-2.55709527340695	-2.59856409156963	1.11128255393652
C	-3.98106867083920	-2.76053001586848	1.23827706331388
C	-4.83605726538169	-2.14324518027402	0.39254045310356
C	-1.03584312031496	-0.09919960259009	-1.95602003857113
C	-0.17047365708135	-0.71419901333079	-1.11807822027949
C	-0.63569184182713	-1.59903715408384	-0.07630143365434
C	0.22760764800890	-2.25486735573123	0.83153530507340
C	-0.30487145430461	-3.04822546248015	1.85109109245868
C	-1.66978580355193	-3.22733411405039	1.98809139809704
C	1.68642014586949	-2.02198976407654	0.79725959036490
N	2.35482837752698	-1.98213133797920	-0.32232041991499
C	3.62349032653254	-1.53671662939184	-0.17250525334713
N	4.37312043221312	-1.80171854860680	0.94006345740759
N	3.73164973361370	-1.89936981974012	2.04287603378389
C	2.38872193366983	-1.64343864374569	1.98374333999675
H	-6.28887250243451	-0.75971136197690	-1.41052939113907
H	-5.41164274033479	0.69913374206233	-3.20638754747515
H	-2.96945466270774	1.00243602197711	-3.48325039904123
H	-4.35328074668053	-3.39495651745107	2.03517446098861
H	-5.90786643000983	-2.27055685307063	0.49794073586569
H	-0.66576483075024	0.56013700413672	-2.73363919067442
H	0.89211136299364	-0.56329515284185	-1.24022659619478
H	0.37337161612380	-3.55016439610566	2.53239035951225
H	-2.06029729663878	-3.86062161158471	2.77661399950971
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H	1.88815217472124	-1.61178269885922	2.94445688431620
C	2.69626019797349	2.82412812961244	-0.56683850941065
C	3.40095280372666	1.45675329536019	-0.68274128337920
C	3.01552798661838	0.59777099512053	0.45290494495833
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C	1.43553175338680	0.94213171095301	2.50921785707784
C	1.04169944214943	2.37870114879461	2.14254706810172
C	0.42418821102061	2.45660796413241	0.76684006995860
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C	-2.57876755065460	2.93699815256167	0.55975652649213
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N	-3.43456245421058	1.89921990424291	0.43365195461813
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H	2.98166969719507	3.43227198379973	-1.43129868338205
H	3.06352320879232	3.34377393501918	0.32206720308384
H	4.48760032933825	1.57645777227444	-0.71448297246424
H	3.10338674917283	0.97734395828174	-1.62235338466267
H	1.89271949028660	0.89880011752945	3.50190403390666
H	0.53672708245864	0.31414889733234	2.54205498305943
H	1.92132947742683	3.02430327155419	2.21171589995844
H	0.30950014437882	2.74768877763015	2.86707344907514
H	0.85195896930702	4.58596057654938	0.54196269172558
H	-1.39205441612932	5.06467132510185	-0.04307694267617
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H	-3.48447149105784	1.45139675761836	-0.46834550927388
H	-3.62118340056258	0.35403924087274	1.85558110845041
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H	-4.01096736666277	2.00020443648376	2.40994602461622
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C	4.11053739054006	-2.23467573719118	-0.73073238758798
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C	3.10443865031165	-3.98961655485774	-2.06482971274942
C	1.93334083326549	-3.25068322927361	-2.18054250965886
C	1.81974055647051	-1.99511779434706	-1.57379141294869
C	2.91991236893048	-1.47125336141576	-0.84908363077207
C	2.82915647798198	-0.18131250195101	-0.24149445190122
C	3.93596867619434	0.32352098916367	0.49030628370640
C	5.12549139209392	-0.47723769797633	0.60429878085728
C	5.21037528004767	-1.69385267629912	0.02181483883640
C	0.60488463624433	-1.22771849607266	-1.62363591461127
C	0.51332150799346	-0.00638825004113	-1.04939311861805
C	1.64149398686863	0.58957388005867	-0.37392941329918
C	1.60632693053541	1.87808135030824	0.20057969583000
C	2.69799070300287	2.34832447832343	0.93358105349465
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C	0.41242009988551	2.73600972408370	0.07015129647434
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C	-0.19604763533414	3.35069749207280	1.20161555324759
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H	5.95961468094563	-0.07520574053688	1.16853018489648
H	6.11401397282453	-2.28704184444746	0.10820427850870
H	-0.25502601266391	-1.65641363427125	-2.12870154876433
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C	-3.56081418496973	-1.88711735477980	1.24123781895596
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H	0.17115819551977	-3.63226902833735	-0.33456305375732
H	1.68307071258810	-2.67452934565936	1.62745919538376
H	2.20549242147345	-4.16025347099167	0.80242715882661
H	1.29861421620570	-4.25861634401284	2.33055820813655
O	-3.24710074922493	4.18637876823627	-2.32083079259937

O	-1.68864644434009	2.88666537761800	-3.23864178463902
H	-0.81643378149864	2.56788811761781	-2.95234503435644

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C	2.82449782741399	1.23147757695644	-0.86363862059911
C	1.93196707208084	1.82538927569345	0.08148285404185
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C	3.87280334561724	2.90843309457762	1.14936758671027
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C	1.57968980562814	3.25206986945423	2.01634065178126
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C	-3.71599124281249	1.37557975894862	0.00230095727410
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H	4.25196014861421	3.55941122290651	1.92940601400044
H	5.78215366587801	2.52447345438836	0.30891174103633
H	0.55176417267038	-0.63718449435440	-2.61468644942589
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C	1.02751935553608	-4.23906253997782	-0.62794188707298
H	0.43150366699836	-1.84800272275239	0.65640349086217

H	-0.79095556279699	-2.24219641415763	-1.32266453114619
O	1.96337765501433	-3.16055362629268	-0.69916369169534
C	2.62227243821479	-2.90469373595890	0.46498070030454
O	2.48593013929727	-3.55555970836636	1.47286996662724
N	3.42508114999000	-1.82823631903222	0.31171950167103
C	4.12303644080870	-1.22343969040338	1.42585742752991
H	-2.98345332126483	-3.55857118264504	-1.34219189038512
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H	-3.17603501528574	-1.10281360470884	-1.50580422709084
H	-1.83461796380220	-1.07176443812751	3.59042958976314
H	-0.51129575725047	-0.43572718056045	2.61733308045668
H	-1.83357351192303	-3.17456198269378	2.27156384875515
H	-0.21295488777565	-2.86700632723024	2.89099356408271
H	-0.75910233672674	-4.68594519230237	0.55257201117575
H	1.49162649098209	-5.07194152399125	-0.09879129320400
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H	3.42565409804142	-1.37828118896916	-0.59037847020747
H	3.66936058239004	-0.26653634910268	1.70484321838584
H	5.17152139543409	-1.05419957224912	1.17403527295295
H	4.06195454673145	-1.90823420426288	2.26959718456617
O	-5.60378232137296	0.55751121114497	-1.20415854894232
N	-3.86956572955792	1.44051603642266	-2.38920501902412
C	-4.46937053012654	1.26580572367348	-3.69530496742326
H	-3.83193216212017	0.65486282478155	-4.33773147210253
H	-4.64287235475417	2.22924644018599	-4.17910591812883
H	-5.42440348678931	0.76321929912160	-3.55380205096852
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C	4.05612135477690	0.68332804831453	-0.28070812014128
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C	3.15509232103591	-1.09794999883224	-2.25558206285051
C	2.24671572204063	-0.20324637158160	-1.67957473785388
C	2.69483989732054	0.70387350709275	-0.68510282223793
C	1.77589173428393	1.61429379012887	-0.07762396532834
C	2.24260956084279	2.50889774894452	0.92120207527078
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C	4.49287281191112	1.60267529807857	0.73595675312107
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C	-0.02202821711432	0.64601906944119	-1.44401765861373
C	0.40627720592811	1.61688698378493	-0.46659234067214
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C	0.00975392581699	3.39961593158897	1.13817448526641
C	1.34175457952893	3.39777046408787	1.51263136255086
C	-1.92581918501660	2.50974563465862	-0.12491820086619
N	-2.40152039670074	2.39097864253403	-1.33689951680572

C	-3.74033801604161	2.16950648457299	-1.36018367302666
N	-4.59744803226812	2.71843070379548	-0.44521901668607
N	-4.13272063045113	2.88660288463729	0.73616378489433
C	-2.86060727911633	2.43736487203712	0.95107931655723
H	5.96812984840484	-0.25199288483590	-0.55448015806706
H	5.17539439684740	-1.81926629654943	-2.29576227176249
H	2.80192395853438	-1.79513788345327	-3.00694394679300
H	3.96642769195694	3.16700565507473	2.06659177538721
H	5.53535037484702	1.58249638842809	1.03416856093014
H	0.50982845964136	-0.93072539852070	-2.75326158594810
H	-1.06534010051495	0.61757295986893	-1.71959681726264
H	-0.67649415811666	4.10213001049041	1.59793811510345
H	1.69683895764055	4.08977969055256	2.26780683441663
H	-4.18746542760325	1.94358021693184	-2.32153272055669
H	-2.53022342727394	2.46797062513425	1.98278930562786
C	-3.53228160316972	-2.21498676009669	-1.19181098653915
C	-3.93515583073759	-0.77235360522409	-1.56146153529157
C	-3.63066061471917	0.14270003593616	-0.44374070092439
C	-3.15477331016321	0.32509633520759	0.68148033998510
C	-2.52737919460287	-0.21263774109511	1.90734862373901
C	-2.36125495725893	-1.73204596932200	1.76530932056981
C	-1.52758472345891	-2.08884823091660	0.55784102098915
C	-2.06708604385103	-2.33487015310291	-0.83096214717878
C	-1.54585335164951	-3.47859600544525	-0.00062786468551
C	-0.25795211392812	-4.21231883525828	-0.32570660240424
H	-0.55767233780605	-1.59742785830310	0.54828728179654
H	-1.38876347253759	-2.00379305338608	-1.61509158237497
O	0.88799968322282	-3.36027432557270	-0.26900962798957
C	1.32244796597378	-3.07985434190407	0.99131643249038
O	0.83642383878878	-3.55261300787830	1.99106685544904
N	2.34849245745462	-2.20324557891303	0.93841528365724
C	2.94122475853721	-1.63213474418111	2.12832522563005
H	-3.75715231043314	-2.86806097706008	-2.04138528573233
H	-4.15440127736583	-2.55353205457298	-0.35881748745547
H	-4.99634626320597	-0.72295138258491	-1.82123128900441
H	-3.37776676594630	-0.45156514687749	-2.45022288200608
H	-3.12784865272268	0.03993827472540	2.78576047625166
H	-1.54283566212731	0.25075392534032	2.04639416839522
H	-3.34806498826584	-2.20025199706002	1.71145634625898
H	-1.86082640218022	-2.12605011871738	2.65519245067875
H	-2.31197869069342	-4.12370030991635	0.42164355056414
H	-0.11965109084033	-5.03363555360104	0.37832465566154
H	-0.26439882123406	-4.60042205233482	-1.34456470677988
H	2.65875580333498	-1.90946280138617	0.02555415518333
H	4.02110645191215	-1.79378083315949	2.13814197985594
H	2.49688798925078	-2.12602751840272	2.99037064172856
H	2.74439499353627	-0.55710360893820	2.18591459026803

5 tco

C	0.24475657998132	-2.55080817514519	-1.65385510834148
C	-0.63437345822158	-2.15964017382778	-0.59613750635906
N	-0.19882694583167	-2.34919615457033	0.62018149848920
C	1.01537318017498	-2.94372090284894	0.68502341578242
N	1.44346950880941	-3.84447931548633	-0.24792352969418
N	1.03757026475443	-3.64338883080025	-1.44859504925842
C	-1.94804192682395	-1.54794941068213	-0.88774203375999
C	-2.49116274407790	-0.48081640858340	-0.13556356095615
C	-3.74109786686690	0.06826385542652	-0.54456823400848
C	-4.43678999030691	-0.46777869327515	-1.66101532387626
C	-3.87541899997642	-1.53388212737244	-2.36535934963786
C	-2.65065072398378	-2.05074515947999	-1.98790326311098
C	-5.70328688880709	0.09524959525021	-2.04286720214024
C	-6.24036199163754	1.13372781227928	-1.36593636774167
C	-5.56101639638915	1.71250174811890	-0.23855902048239
C	-4.31204420478855	1.16982612560287	0.16416877444028
C	-3.63290600556195	1.73007885891164	1.27457892651157
C	-4.20221231632919	2.81110569694288	1.95458381529578
C	-5.42308815861962	3.33605945334922	1.55353676779108
C	-6.09745113221050	2.79207614872529	0.46763031867666
C	-1.83273099210880	0.10735800786130	1.00678098132101
C	-2.37638312949539	1.15716836988389	1.66568080104925
C	1.75057545330214	-1.01968355041847	-1.34439794943647
C	1.00114374874425	0.25948759805387	-1.61497448624124
C	2.01754599424096	1.36519575519236	-1.96277092938214
C	3.17233893663845	1.48086775522863	-0.96272908233057
O	3.65470914176335	2.83680525851263	-1.13393638406008
C	4.42308745878124	3.29023958785709	-0.15009654485575
O	4.73206012606884	2.68578738931946	0.84199776974679
C	4.35060480293461	0.48811089350631	-1.14926678029746
C	4.60869454672955	-0.47627664064289	0.02080580970025
C	3.69361684994459	-1.72020109533813	0.04735669910820
C	2.27183634073416	-1.25551782558332	-0.08709291102771
O	4.79800229028232	4.53307014984526	-0.44127096421012
C	5.63575610159703	5.14233387167218	0.54230866662348
H	-7.05180526539810	3.20196512233750	0.15565087806528
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H	-7.19591654100666	1.55285919555529	-1.66171649546348
H	-1.86435457613801	1.58070955972544	2.52293021514112
H	-0.90773303907100	-0.32735054506852	1.35850379842679
H	-2.23702654488764	-2.89089792670785	-2.53361704328657
H	-4.40933034934746	-1.95568419017031	-3.20922230177166
H	0.00908311338400	-2.33986610568648	-2.69000423098817
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H	0.28579714092984	0.16239068899970	-2.43644633727676
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H	1.50101399984100	2.32692070180988	-1.99041862584091
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H	4.21740335436320	-0.07363190088116	-2.07843599687273
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H	5.64678420623507	-0.81631915172910	-0.02284126346005
H	3.87120277857988	-2.27793864806245	0.96981044370326
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H	5.12382343480938	5.18513112261890	1.50357950497615
H	5.83981961789721	6.14242959582048	0.17061029795393
H	6.56137515482607	4.57760070386448	0.65459541110637
C	1.62564574242773	-2.99096919629592	2.06085917527090
O	1.41926950919158	-2.14658397558231	2.88835486516839
O	2.43924409069985	-4.02886735913297	2.22955074327620
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H	3.67112861674239	-3.18078589229150	3.66974692347479
H	3.71552390814841	-4.96325170419688	3.47791198339330
H	2.33591676819354	-4.16793046780581	4.29777065905232

6 tco

C	0.34145818682839	1.75039736066467	2.00605298253244
C	-0.70750898010251	1.77955375091460	1.02638572191733
N	-0.46925855826607	2.45706804121924	-0.06322709679760
C	0.73750886840898	3.06745865220946	-0.07237690037741
N	1.32952867196273	3.52963858956347	1.06485236432083
N	1.12244223403638	2.85868651396771	2.13937729010711
C	-1.96666634849400	1.03903356091503	1.24517347784119
C	-2.64017808575911	0.34509402375291	0.21224300032841
C	-3.81197352294526	-0.39439133319468	0.54487041756777
C	-4.31058226145139	-0.40127594376811	1.87503325351961
C	-3.62869907675063	0.31493284858796	2.86074203622572
C	-2.47379804864417	1.00714646153361	2.54846431700455
C	-5.50284618782858	-1.14542276220958	2.17941574330007
C	-6.15132455395888	-1.84887510923617	1.22524368110469
C	-5.67067562911706	-1.87743507687177	-0.12938708745353
C	-4.50017593162550	-1.14394943760077	-0.45846393650996
C	-4.01564400264234	-1.16333622389369	-1.78977012259294
C	-4.69630132588378	-1.90731644450422	-2.75830915042159
C	-5.83894149093126	-2.62276293710161	-2.42782782808646
C	-6.32323284756904	-2.60824633255439	-1.12578993369313
C	-2.18250906766236	0.31270317337299	-1.15635238126887
C	-2.83549251905901	-0.40736322006072	-2.09763711778005
C	2.03975117388325	1.25729617293445	-0.27051873554798
C	3.43995918606748	1.76903230594530	-0.46957286563157
C	4.28490073494513	0.65440972477926	-1.12199240068642

C	4.17698845273980	-0.69692177476964	-0.41153911369606
O	5.38790270993868	-1.39832430998332	-0.78596391944047
C	5.69800250426248	-2.43700853327077	-0.01836946695773
O	5.07059001482418	-2.82711219808691	0.93032316269695
C	2.94286402238799	-1.56503875573805	-0.77204738724365
C	1.98971972443333	-1.88898356935158	0.38981837581737
C	0.97620604229668	-0.77237076897053	0.72036850075286
C	1.72736727627118	0.52584902024929	0.86105270447490
O	6.82521744214206	-2.97870942718333	-0.46994774313877
C	7.27472273179545	-4.11402018212362	0.27120217921906
H	-7.21631043266592	-3.16727952525390	-0.86908368780131
H	-6.35669587735268	-3.19320807181505	-3.18944045859331
H	-4.32084573229664	-1.91614845786765	-3.77549863110617
H	-5.86745870693475	-1.12941978580798	3.20040560341959
H	-7.04791094385657	-2.40981346024657	1.46516290167498
H	-2.47469026433595	-0.41216674187397	-3.12038494101255
H	-1.32472245490821	0.90688776017048	-1.43580314390819
H	-1.96563838576419	1.56731721525889	3.32502478930032
H	-4.01161865046168	0.32361499305854	3.87472042909472
H	0.26567046297931	1.13321965088972	2.89273832063539
H	1.48383517937461	1.03362430783582	-1.18017238291676
H	2.44562130548804	0.56558551948750	1.67857343273151
H	3.48326276622243	2.65209881299784	-1.11051135283051
H	3.86744489191429	2.03798645821550	0.50154635678252
H	5.33445133967486	0.95544419337351	-1.11484457400779
H	3.99168797687870	0.53473847804778	-2.16929348271160
H	4.22028518503776	-0.55367185881184	0.67214636898181
H	3.32561117988394	-2.50888982086220	-1.16569175991727
H	2.39100309005304	-1.09857709017177	-1.59340491120016
H	2.59081182920383	-2.12504084538195	1.27229348731440
H	1.42591305750621	-2.79298498224998	0.14598351222122
H	0.42512611998831	-1.03949703779693	1.62660654705803
H	0.24805801476857	-0.68481475654674	-0.09325404174917
H	8.19164401606905	-4.43383908872003	-0.21551039076690
H	6.52748534213252	-4.90692735439255	0.24135288130769
H	7.46522792364566	-3.84042325427297	1.30896584015942
C	1.16893251485579	3.74707425952012	-1.35224045094600
O	0.80079710382863	3.38757766744717	-2.42865596887016
O	2.04534132836585	4.73775848270299	-1.16716244231507
H	2.19127625317193	4.83254074272975	-0.21060726543531

7 tco

C	0.74243743826940	2.33073381577530	1.88881907969262
C	-0.13974092958912	2.19076366956261	0.76923443852904
N	0.36226716555642	2.45004241530222	-0.40678465640710
C	1.65351661780528	2.85849733247847	-0.37797972020561
N	2.16084424437979	3.57538704872054	0.66787739708562
N	1.68907758506901	3.31065543532998	1.83174138753716

C	-1.53295569523879	1.73253629426357	0.95260029621207
C	-2.16053485083885	0.81881062406965	0.07441991400313
C	-3.48570143353108	0.39090268291269	0.37602142405623
C	-4.16992117901045	0.90073377441739	1.51144781609598
C	-3.52080968000785	1.81445915844813	2.34389814686712
C	-2.22372328414240	2.20765124141059	2.07188980824967
C	-5.51336956272169	0.46474098178845	1.78129270045818
C	-6.13230590621894	-0.43178139545459	0.98201469054232
C	-5.46692675251586	-0.98315891636561	-0.16705225466937
C	-4.14298222572405	-0.56261997953635	-0.46094341243425
C	-3.47380639896863	-1.09989803082255	-1.58837240337771
C	-4.12798960761643	-2.03745733787271	-2.39323488274596
C	-5.42298766995509	-2.44227782338563	-2.09958729067534
C	-6.08799831097655	-1.91994259289896	-0.99733426745485
C	-1.51470167393400	0.26117209111255	-1.09001317786360
C	-2.13886632190653	-0.65349907816938	-1.86725713142414
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C	1.07394671230458	-0.52685149716348	1.54804132305166
C	1.89318920437159	-1.81362765770126	1.76580302156040
C	3.01108155132719	-2.00221981364304	0.73065449168500
O	3.35230487878981	-3.41091396624500	0.67486919057960
C	2.51517120398747	-4.17618897922603	-0.01899419480930
O	1.52416921242328	-3.80868132782941	-0.59015054625897
C	4.34244695169434	-1.27218835153991	1.02069776758149
C	4.77336714470642	-0.22579322780787	-0.02045367651983
C	4.08246394021553	1.14995687954862	0.11431777293351
C	2.59918709921246	0.92729514245116	0.20112058212041
O	2.95966567927794	-5.43036308136035	0.01902997808918
C	2.15061956628526	-6.36194679225769	-0.70041666611897
H	-7.10001790088571	-2.23576338122695	-0.76885926259322
H	-5.91774049557512	-3.16864607755711	-2.73311423600612
H	-3.60874117271985	-2.44502359050164	-3.25352566795669
H	-6.01822170466074	0.87578957619291	2.64854457460757
H	-7.14544874315888	-0.75542562827372	1.19455991783852
H	-1.63004571256402	-1.06302096506854	-2.73289032848984
H	-0.52757884385659	0.60811030784036	-1.35975029625094
H	-1.73878415496895	2.92810572319592	2.72075491963644
H	-4.04300943580925	2.21441158410103	3.20565315939289
H	0.43451062401966	2.04539479838780	2.88737254550273
H	2.63052062884595	0.84126225817167	2.30483957985736
H	2.13401462087302	0.50907368577861	-0.69087585206823
H	0.36597854674958	-0.40793541150701	2.37291432358767
H	0.49296299211781	-0.62925491770140	0.62612786058818
H	1.21005931844186	-2.66284733750252	1.70081108213684
H	2.33251344958719	-1.81823603381842	2.76858457243240
H	2.63145808053410	-1.73139082516111	-0.25732721477532
H	5.10774379941778	-2.04895268012717	1.06484508521396
H	4.31229990490711	-0.81525984295529	2.01417208009522

H	4.58326303213279	-0.62181517224750	-1.02353636628076
H	5.85366613071981	-0.07506662398175	0.05343850593606
H	4.36312578395238	1.77150359345271	-0.73918119312804
H	4.42841234798128	1.65277714391211	1.02326055230248
H	2.12547468848162	-6.10365994959831	-1.75926722164551
H	1.13318715253594	-6.36371848984439	-0.30984941858072
H	2.62049873269159	-7.33035340612777	-0.55389122178416
C	2.33621966492694	3.01071188207085	-1.72192990334050
O	2.07874691330614	2.25624287051279	-2.63653314481729
N	3.24904147700073	4.00561376111741	-1.76202525380244
C	4.03088051525253	4.28579236785236	-2.94840684098048
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H	3.73731844441174	3.56829694505236	-3.71213863711345
H	3.37716663988243	4.54102995544357	-0.91544940440084

10 tco

C	0.37377309406036	2.73793259936897	0.79137008089045
C	-0.67044052792147	2.33881669673141	-0.09565281485609
N	-0.44858728409514	2.49589070461861	-1.37568253557739
C	0.76349190136116	3.03481145657719	-1.65667705467877
N	1.38046910152593	3.93455496799562	-0.83084320391892
N	1.16427348304190	3.78824066668664	0.42563652477284
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C	-3.76635499147864	-1.71415755844737	-1.29094683235115
C	-4.38402993927157	-2.84752307330267	-1.82719386382567
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C	-2.59310732478766	-1.13484219154940	-1.87947100126255
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C	4.27406301028787	-0.42440401129495	-0.49974707873910
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C	5.91529587107879	-1.74612221308250	0.52647701981682
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H	2.46647500704458	-1.40350256259949	-1.23071434089263
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C	1.94902414822330	1.87107169012838	0.27765569117874
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C	4.32365312204638	1.38460415191670	0.59007131250724
C	4.01481581091052	0.06576980617295	-0.09282809075103
C	3.00664910128679	-0.95270877434075	0.40580909104423
C	4.48460401841672	-1.25575796336940	0.44743783909122
C	5.09606056659321	-2.25724324881852	-0.48688071660824
H	4.03290285442434	0.13816980288577	-1.17883931169452
H	2.47047415316748	-1.45669445660610	-0.39242591199627
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O	2.96252034428109	-3.83425241219719	-0.96040832117064

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C	4.19186385323853	1.48742472818094	0.03995920263029
C	3.80710806502763	0.16770250747648	-0.60186752660377
C	2.85029021332885	-0.83825207932799	0.01185604240532
C	4.32233579282934	-1.14631776163094	-0.08783271333880
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H	2.23373206300569	-1.35215891523080	-0.72243541209085
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O	5.99638819662531	-3.48462998053662	0.94285517446249
O	4.60331002932309	-5.22831701311031	0.65153860984314
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H	-4.81040140578894	1.32566281523990	3.20579561272094
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O	1.70245316704251	5.08432493159114	-1.82568943137637
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H	1.38567813508933	-2.22719731623358	-0.29520641565442
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H	-7.88353672889615	-1.05945587613038	0.73148157752613
H	-2.06391650669147	-0.87888850836494	-2.73763388901262
H	-1.16132839413792	0.75402004899236	-1.17608651510513

H	-2.85527560472117	2.88227611301016	2.82168124147690
H	-5.13331265074301	1.99485227413606	3.10581796969892
C	1.47174363597050	3.47958468888156	-1.36076325924876
H	-0.60073391498892	2.10241296737033	3.08567741402330
O	2.60123540278350	3.91540857587934	-1.36523238667054
N	0.76275017639117	3.14762205699813	-2.46918901189341
C	1.28491951773392	3.37791415707000	-3.80003779258183
H	1.18404130236595	2.48024952127868	-4.41228381931575
H	2.33910133060861	3.62983605820126	-3.70095397417450
H	0.76954852841495	4.20571901806814	-4.29274317874259
H	-0.20790834617494	2.90659562811666	-2.33209506064317

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C	2.19751591616999	0.69278935718219	1.49433132108172
C	0.80272769282261	1.28911678695990	1.18942694845803
C	1.04036563217915	2.61092805119421	0.50996941680673
C	1.41516167908722	2.63700145766452	-0.80912032708775
C	2.66083374850990	3.38547886759332	-1.21007815663297
C	3.85011676961673	2.68063419292717	-0.51231544490388
C	3.77850749967514	1.17143123981682	-0.65238654597577
C	2.98279613616830	0.26259635842700	0.26797447103012
C	4.48780528822948	0.24452843954481	0.29396162306167
C	5.22388155556721	-0.94154977203996	-0.24139644037331
H	3.77328752248190	0.83957503436617	-1.68889762093707
H	2.53413840451636	-0.58573524243611	-0.24441790483523
O	5.17823178206489	-1.96736972115796	0.76623021725597
C	5.70781853637690	-3.12958013621629	0.39798532117920
O	6.18364242411480	-3.37626046186313	-0.67610316107225
O	5.62092498548291	-3.97836161620200	1.41938922134165
C	6.15453314369633	-5.27561927099676	1.15322995376947
H	2.08575161067363	-0.18340237217586	2.14011287894639
H	2.77293315748099	1.42515814170195	2.07071540252255
H	0.23894516908296	1.39589341394856	2.11994134865766
H	0.24363480865339	0.61151342361255	0.53553741369533
H	1.45100720354227	3.39160193516192	1.15086087455436
H	1.19487419397839	1.74432691144139	-1.39120151388897
H	2.79485319132924	3.37122033944888	-2.29534440614913
H	2.60517574335210	4.43064616111081	-0.89504206678395
H	3.83698446792180	2.94746051041063	0.54894847918948
H	4.79957215710727	3.04249394288617	-0.91909315636559
H	4.94389744245441	0.71125326277864	1.16262941734693
H	4.75647427197187	-1.31861636984203	-1.15469898059407
H	6.26960203806327	-0.71603942000128	-0.46429092874873
H	7.21033997998124	-5.20655399052140	0.89091486197714
H	5.61407276236415	-5.74971662533712	0.33374524828556
H	6.02445180915048	-5.83774883143481	2.07354041258736
C	-4.78607880736153	-2.62888073516580	0.35622380335660
C	-4.82427578479008	-3.97149416098689	-0.02933793368514

C	-3.88797493766479	-4.48138239598663	-0.91951914487232
C	-2.89762406203217	-3.66064440041663	-1.44231066718303
C	-2.82682605482091	-2.31170043931300	-1.08306532976343
C	-3.77815188540634	-1.78188243809461	-0.17487616245638
C	-3.71839729253329	-0.40605615949276	0.20671974145094
C	-4.67006232274910	0.09868336171578	1.13267332609008
C	-5.68419270276005	-0.77988041988522	1.65037645181056
C	-5.74042689164691	-2.07857443522030	1.28122992789996
C	-1.81896471851609	-1.43297625907607	-1.60584531874129
C	-1.76484324350069	-0.12705341732803	-1.25758861689947
C	-2.71256017764114	0.44495397567316	-0.33238397974801
C	-2.66198874378000	1.79081325487341	0.09297179202139
C	-3.60018272142282	2.25798979418548	1.01813593327508
C	-4.59340399733025	1.43716749602292	1.52187876482319
C	-1.62245026481354	2.74137291495046	-0.36352121430762
N	-1.23135712904262	2.80921004794491	-1.61189213987272
C	-0.26721935120911	3.73400688737364	-1.83274349379385
N	-0.14598092271998	4.87679526349754	-1.10059369716677
N	-0.52882710231846	4.81390756179945	0.12718615484085
C	-0.98481071956027	3.61154324372978	0.56612908467289
H	-5.59636368671005	-4.61482785544212	0.37819580378167
H	-3.93080153347170	-5.52479018211279	-1.20763293366157
H	-2.16834418221895	-4.05968570552923	-2.13863883833064
H	-6.40402064567776	-0.37195912268241	2.35138969501943
H	-6.50668721556628	-2.73463668610328	1.67953702923387
H	-1.09542302001520	-1.84012043293259	-2.30397965522002
H	-1.01856795637980	0.52001106771871	-1.69428131673873
H	-3.56384971951012	3.29839996994981	1.32039679073116
H	-5.32068852483317	1.83043968921876	2.22307943676149
H	0.15614331669264	3.78055159896320	-2.82928437647556
H	-1.18930063255673	3.54877559839846	1.62862283164870

Luminescent properties

Samples were prepared in ethanol at 10^{-6} M concentration range to elicit an absorbance of around 0.1 to prevent inner filter effects. Absorbance at 350nm was measured on a Jenway 7315 spectrophotometer in a 4cm path length quartz cuvette between 300 and 400 nm for each compound, and optimum excitation of 350nm selected for investigation in fluorescence studies.

Fluorescence emission spectra were collected on a Horiba Fluoromax F4 in a quartz cuvette (1cm path length) with excitation wavelength set to 350nm, scan range of 360 to 685 nm with 2nm entrance and exit slits, corrected for instrument response and incident light flux. Excitation spectra were collected between 250 and 380 nm with emission monochromator set at 390 nm and 2nm slits.

Emission spectra were gathered over a series of concentrations for each sample and integrated over the range of 360-550 nm to determine photoluminescence quantum yield as described in Horiba application note (https://static.horiba.com/fileadmin/Horiba/Application/Materials/Material_Research/Quantum_Dots/quantumyieldstrad.pdf) compared to 9,10-diphenylanthracene (DPA) as the relative standard[3]. All solutions were in the same solvent, so no refractive index (η) correction was necessary. Plots of absorbance vs integrated emission were generated and the gradients (Grad) compared to DPA to elucidate relative quantum yield of fluorescence (Φ).

$$\Phi_x = \Phi_{std}\left(\frac{Grad_x}{Grad_{std}}\right)\left(\frac{\eta_x^2}{\eta_{std}^2}\right)$$

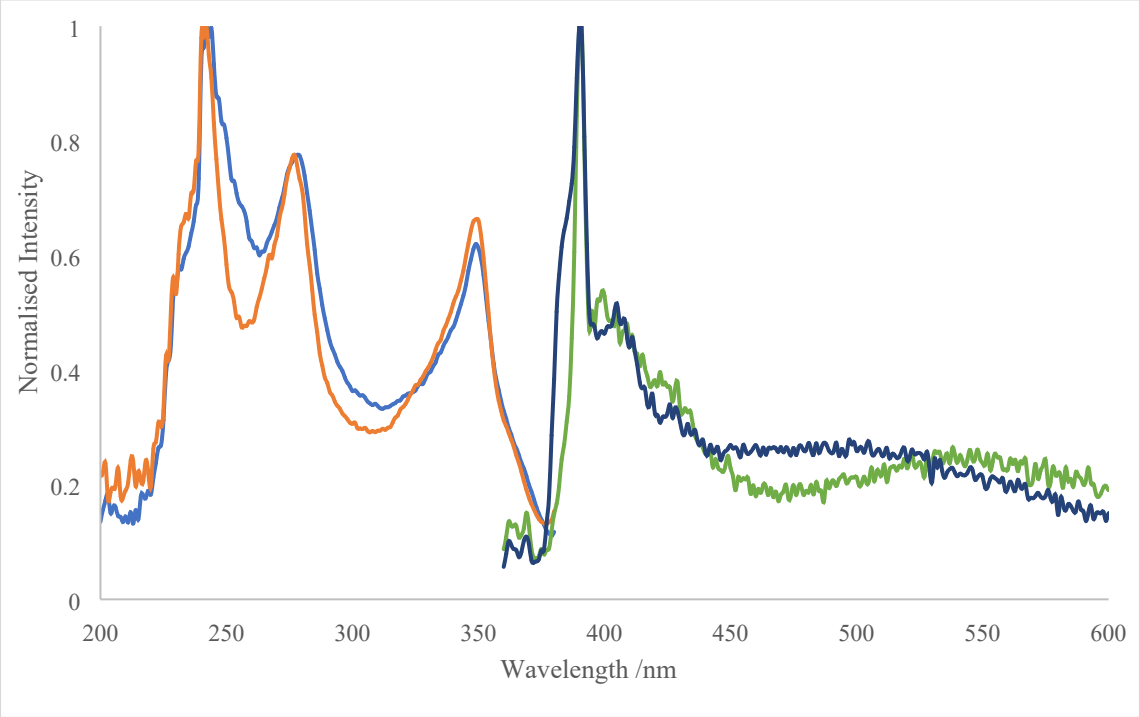

Figure S38; normalised excitation and emission spectra for compound **7** (blue, green) and compound **10** (orange, dark blue) showing a Stokes shift of around 40nm when excited at 350 nm. Note also the emission at around 550 nm attributed to the excimer formation of pyrene derivatives.

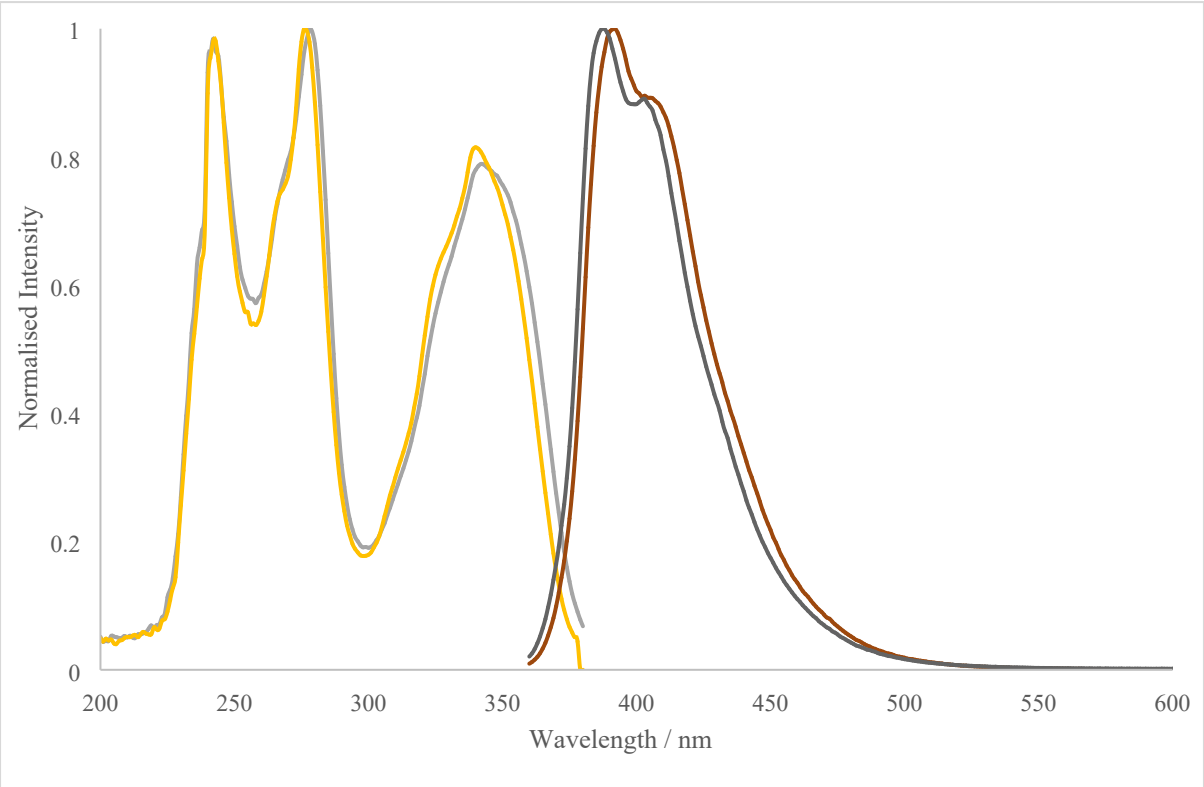

Figure S39; normalised excitation and emission spectra after the reaction of triazines **7** and **10** with **BCN-C10** (20 equivalents) in ethanol to give pyridine derivatives **15** (grey (ex), red (em)) and compound **14** (yellow (ex), dark grey (em))

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