Photochemical [2+2] Cycloadditions of Naphthalene Acrylic Acids: Templated and Untemplated Photoreactivity, Selective Homo/Heterodimerizations, and Conformational Analysis

Supporting Information

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X-ray Crystallographic Analyses of Compounds 6a and 15a:

Suitable crystals were selected for data collection which were performed on a Bruker diffractometer equipped with a graphite-monochromatic Mo-K_α radiation at 293 K. We used the following procedures for our analysis: solved by direct methods; SHELXS-2013 [1]; refined by full-matrix least-squares methods; SHELXL-2013 [2]; data collection: Bruker APEX2 [3]; molecular graphics: MERCURY [4]; solution: WinGX [5]. Details of data collection and crystal structure determinations are given in Table S1.

Table S1. Crystal data and refinement parameters for **6a** and **15a**.

	6a	**15a**
Empirical formula	$C_{36}H_{24}O_4$	$C_{36}H_{24}O_4$
Formula weight	520.55	520.55
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1$	$P2_1/n$
a (Å)	7.9745 (7)	8.8325 (7)
b (Å)	12.9911 (10)	21.7745 (18)
c (Å)	13.0553 (11)	13.8399 (14)
β (º)	104.833 (3)	102.856 (2)
V (Å^3)	1307.43 (19)	2595.0 (4)
Z	2	4
D_c (g cm^{-3})	1.322	1.332
μ (mm^{-1})	0.09	0.09
θ range (º)	1.6-28.4	2.5-26.5
Measured refls.	32579	58261
Independent refls.	6499	5346
R_{int}	0.032	0.063
S	1.03	1.02
R1/wR2	0.041/0.093	0.050/0.112
$\Delta\rho_{max}/\Delta\rho_{min}$ (eÅ^{-3})	0.23/-0.19	0.16/-0.25
CCDC	2426760	2426761

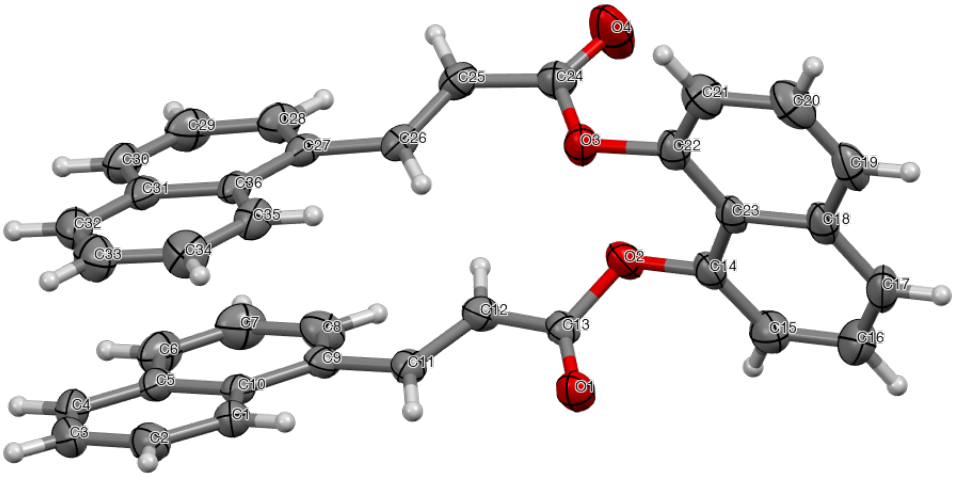


Figure S1. The molecular structure of **6a** showing 40% probability displacement ellipsoids and the atomic numbering.

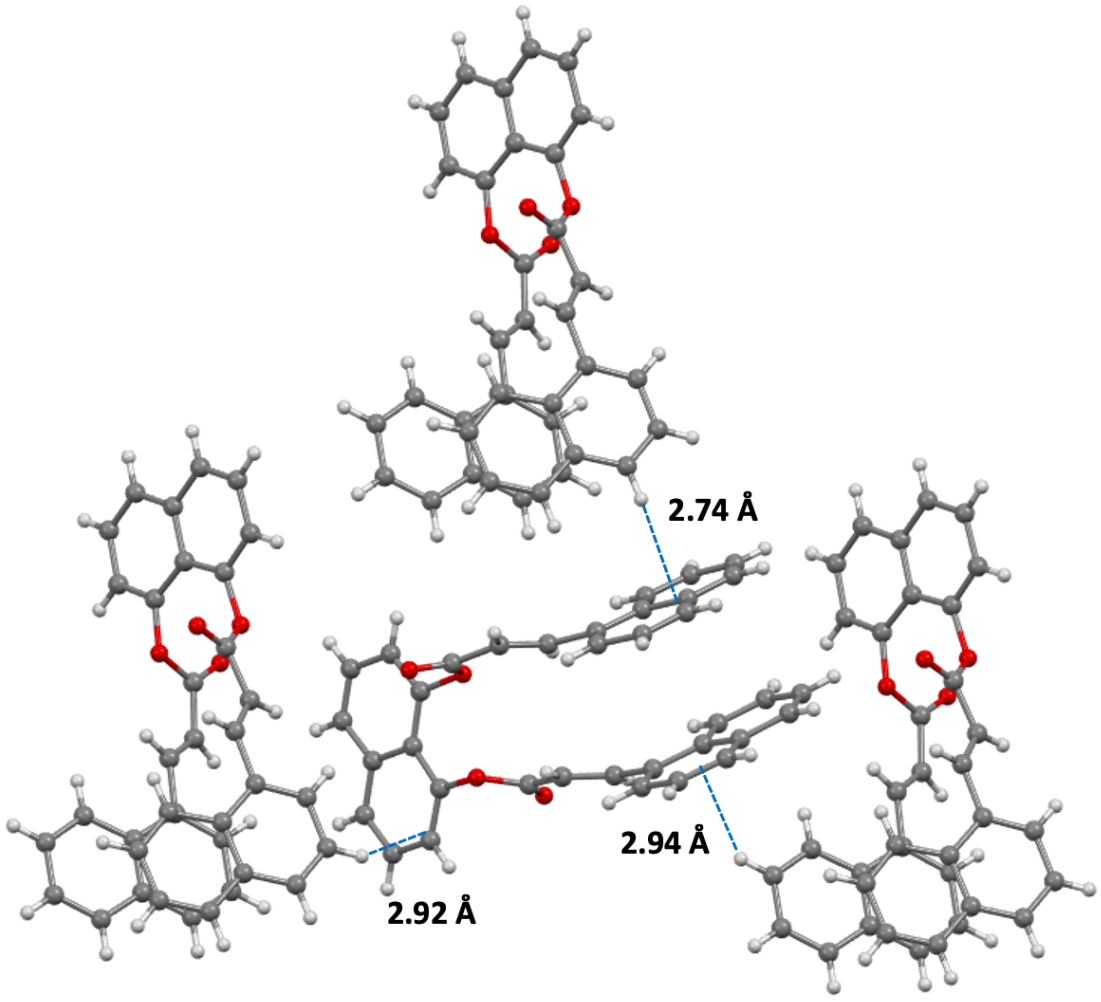


Figure S2. CH–π interactions in the crystal structure of **6a**.

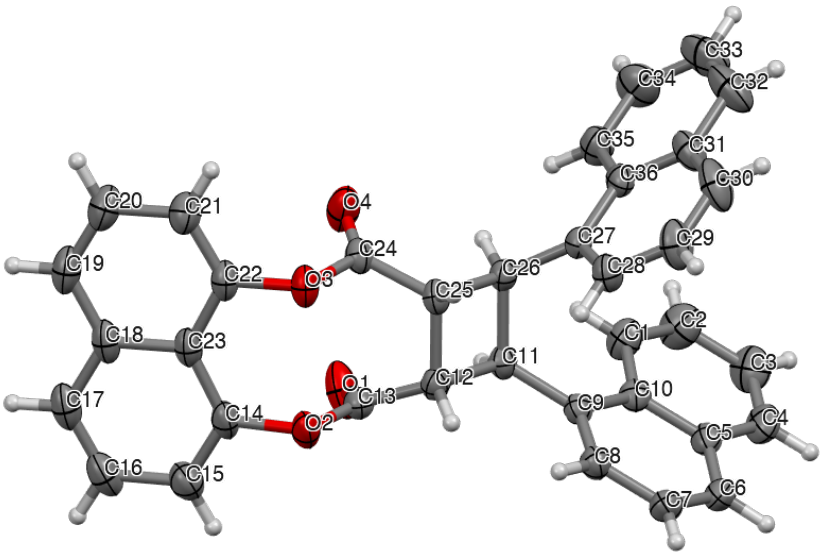


Figure S3. The molecular structure of **15a** showing 40% probability displacement ellipsoids and the atomic numbering.

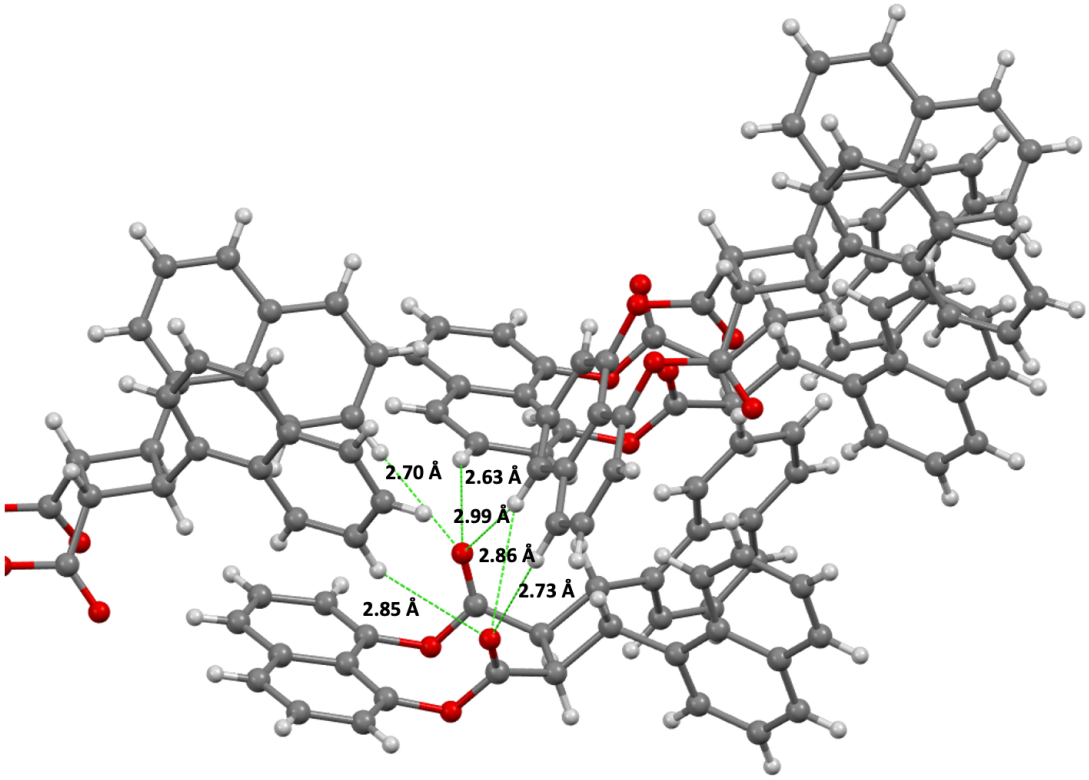


Figure S4. CH–O interactions in the crystal structure of **6a**.

Daylight-Mediated Cycloaddition of Diester 6a:

Diester **6a** (33.1 mg, 0.063 mmol) was dissolved in 1.0 mL of $CDCl_3$. A portion of this solution was transferred to an NMR tube, and the tube was placed in front of the window inside the laboratory. Conversion (%) values were determined periodically for 15 days (between the dates 16.01.2024 and 31.01.2024) by ^{1}H NMR spectroscopy. For the calculation of conversion values, the integration of the signal at 8.61 ppm for **6a**, and that of the signal at 5.68 ppm for **15a** were utilized. At the end of 15 days (360 h), 96% conversion was determined.

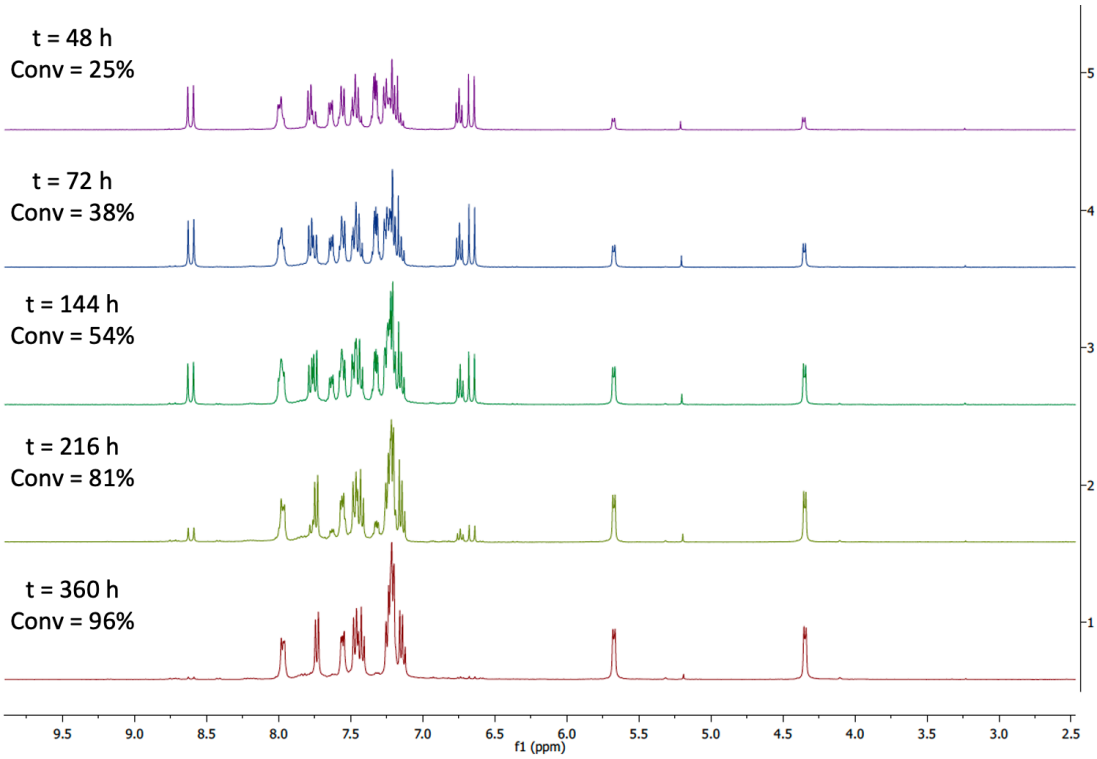


Figure S5. Stacked ^{1}H NMR spectra for the cycloaddition of **6a** under daylight in $CDCl_3$.

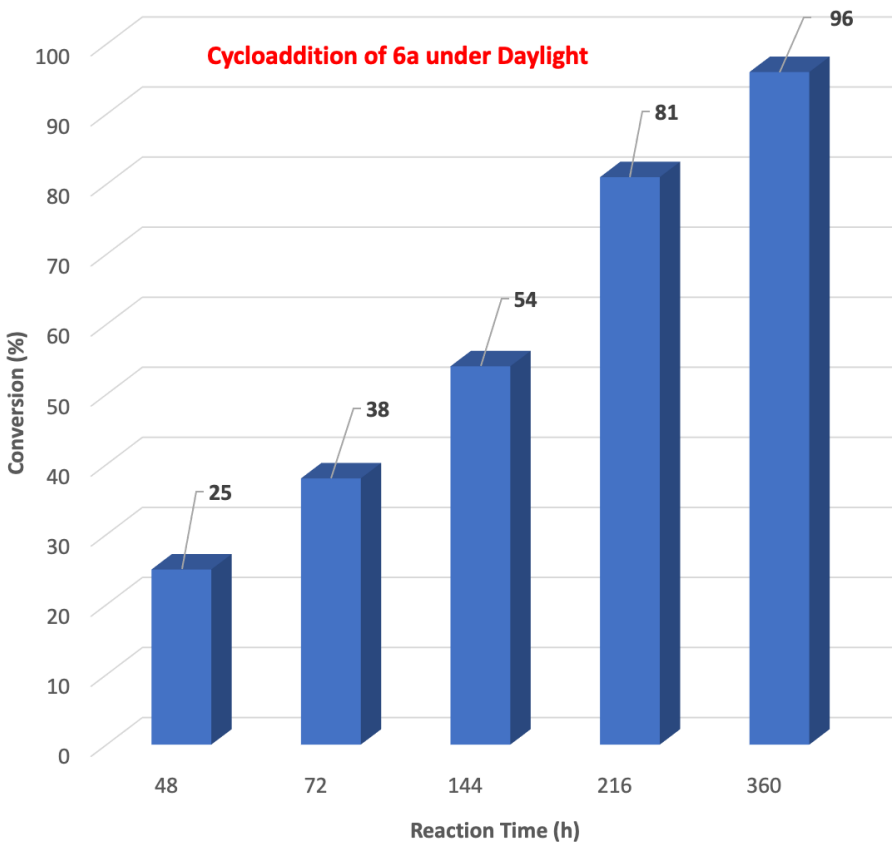
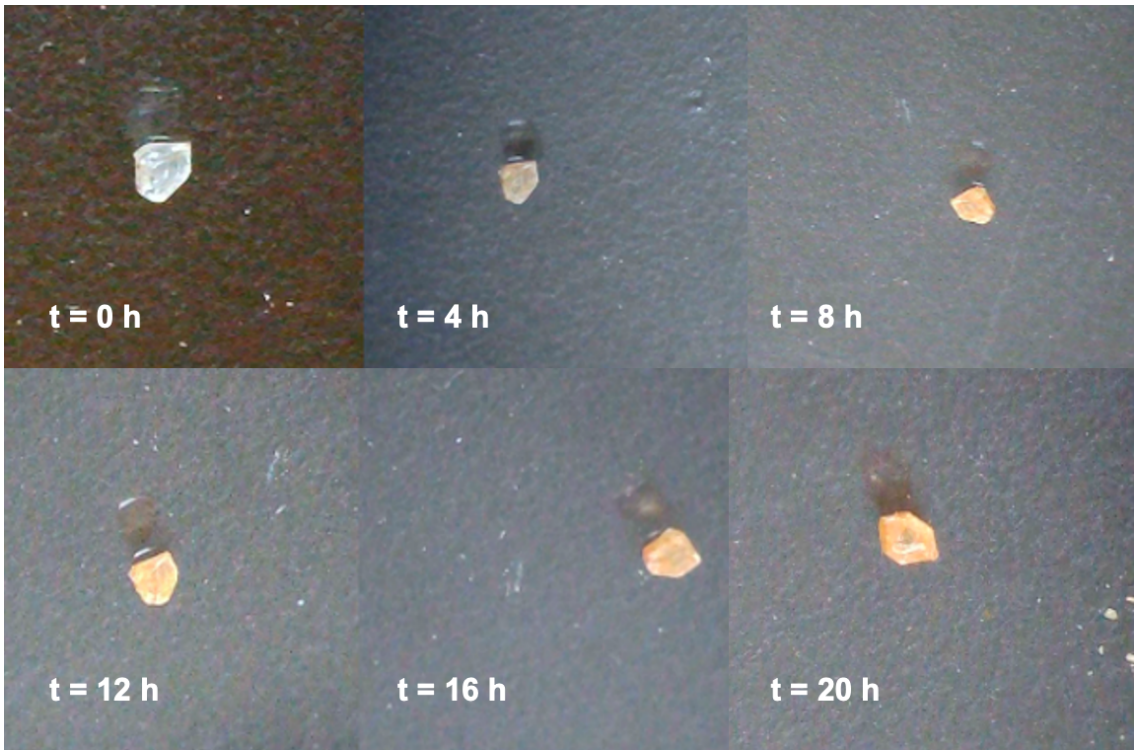


Figure S6. Time dependence of the conversion values for the cycloaddition of **6a** under daylight.

Irradiation of Crystals of Diester 6a:

Crystals of diester **6a** were gently picked and placed on a quartz microscope slide. Unlike the powder samples, a second slide was not used to squeeze the crystals. For 20 h, crystals were irradiated with 365 nm UV light. Every 4 h, they were turned gently upside down to provide equal light distribution. At the end of the irradiation period, crystals were directly dissolved in $CDCl_3$ without applying any purification, and conversion values were calculated via ^1H NMR analysis.

a)



b)

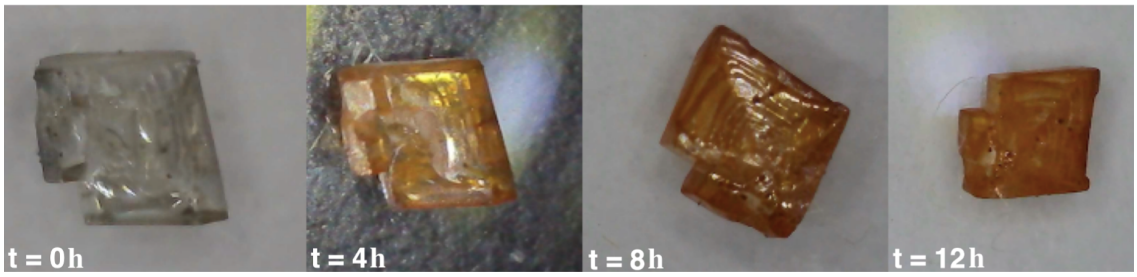


Figure S7. Change of the appearance of crystals of **6a** over time upon irradiation.

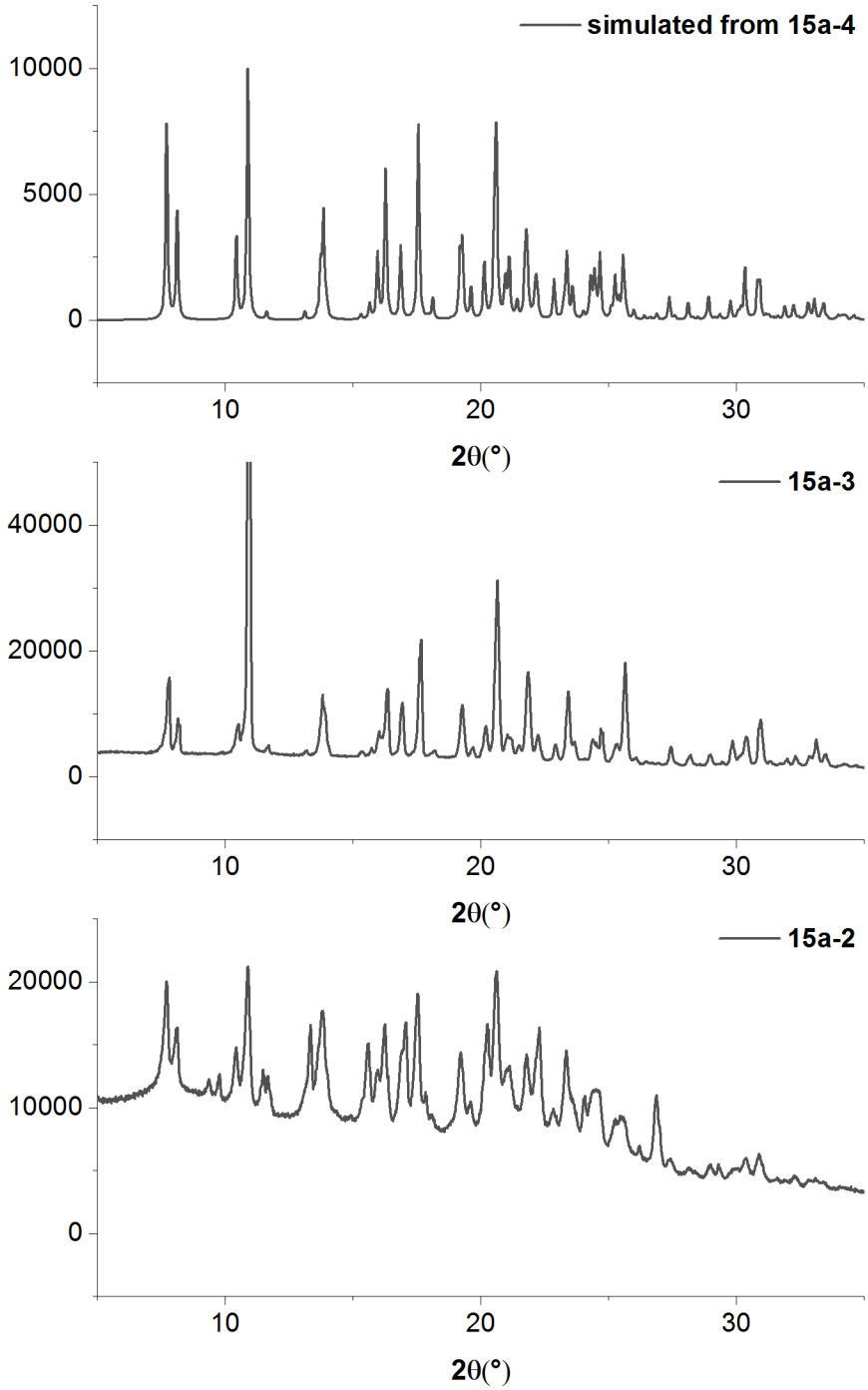


Figure S8. Powder XRD spectra of **15a-2** and **15a-3**, and the simulated powder XRD spectrum of **15a-4** based on its single-crystal XRD data.

ATR-IR Spectra of 6a and 15a:

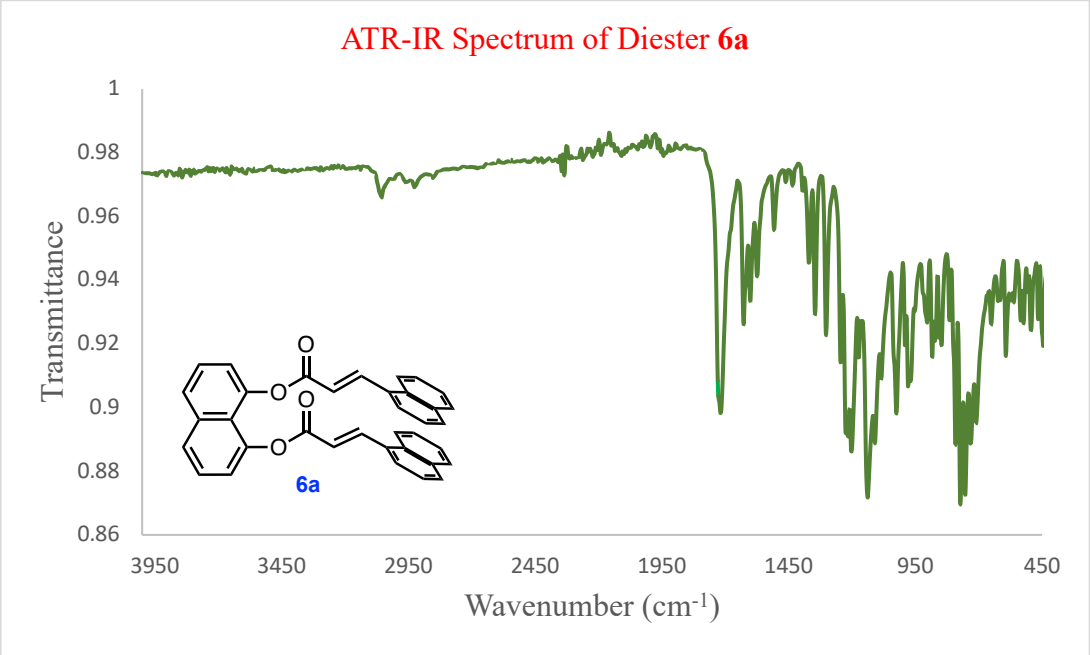


Figure S9. ATR-IR spectrum of diester **6a**.

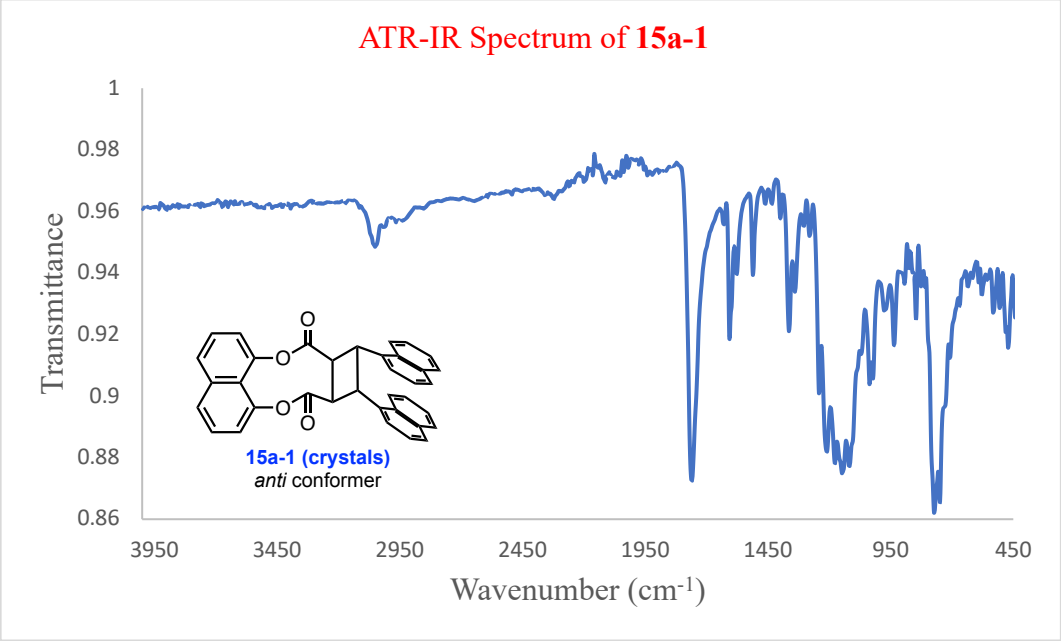


Figure S10. ATR-IR spectrum of **15a-1** after irradiation of the crystals of **6a**.

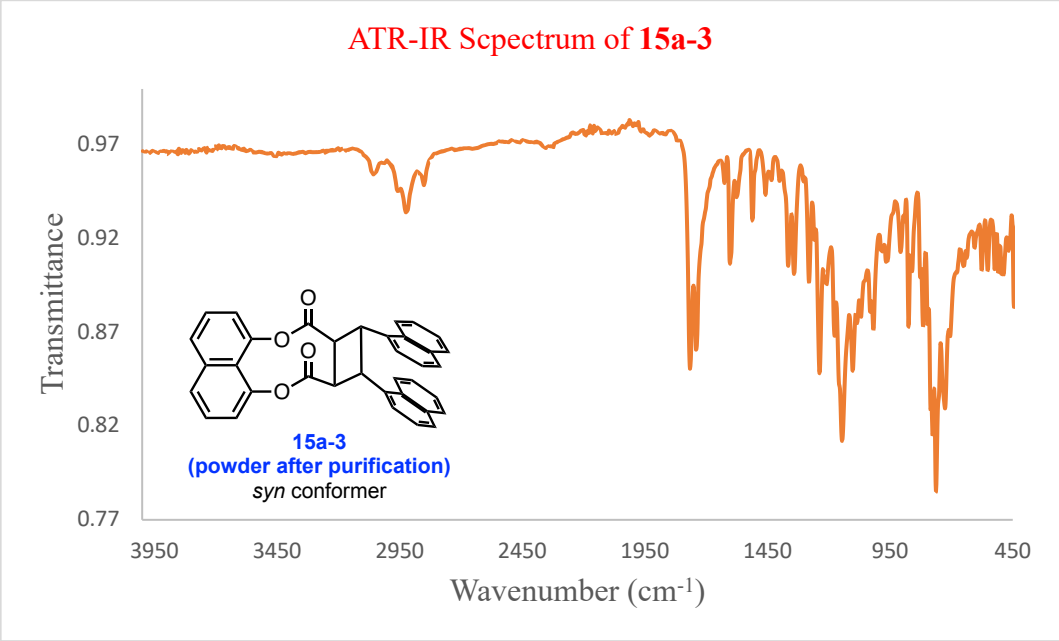


Figure S11. ATR-IR spectrum of **15a-3**.

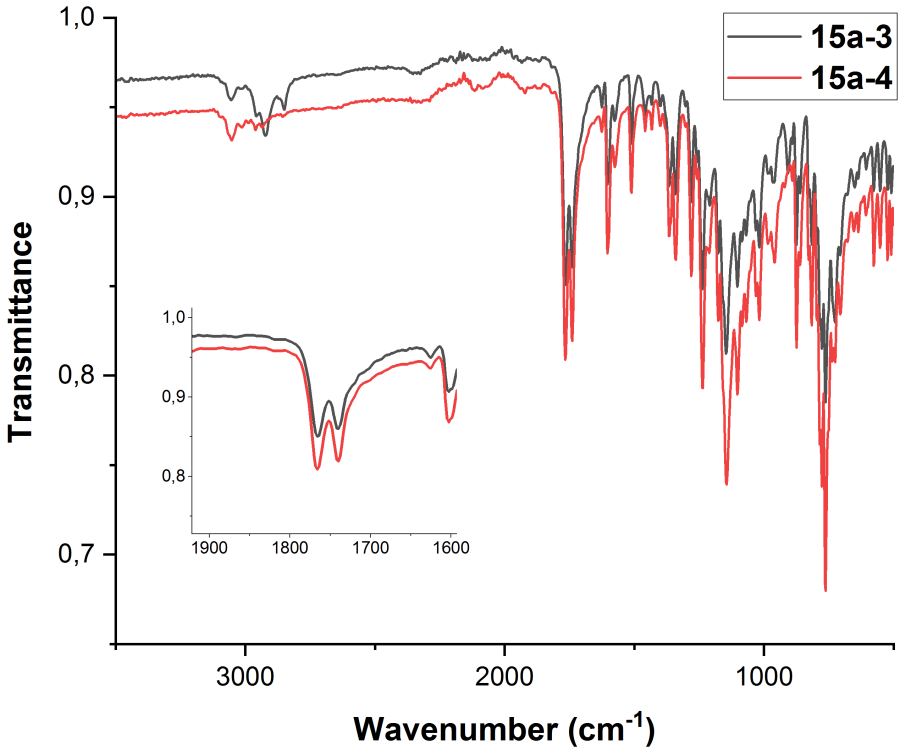


Figure S12. Overlay of the ATR-IR spectra of **15a-3** and **15a-4**.

UV-vis Absorption Spectra of Compounds 6a, 9, 10 and 15a:

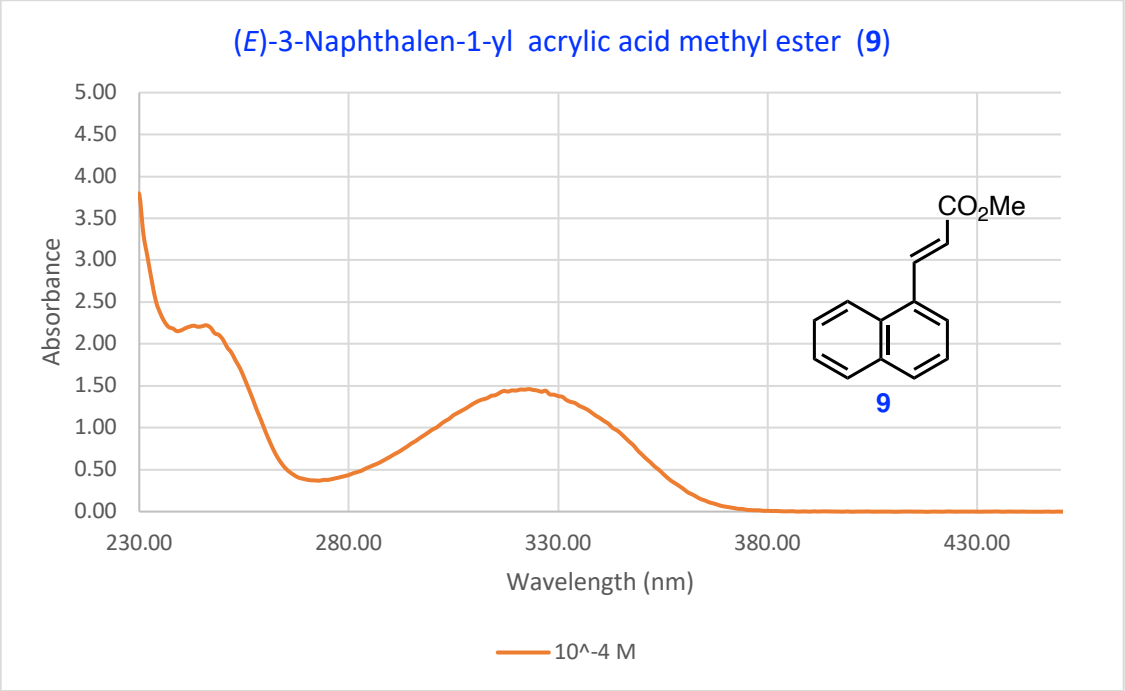


Figure S13. UV-vis absorption spectrum of compound **9** in MeOH (1×10^{-4} M; $\lambda_{max} = 323$ nm, absorption tail up to ca. 378 nm); ε (323 nm) = 1.46×10^4 M^{-1} cm^{-1}.

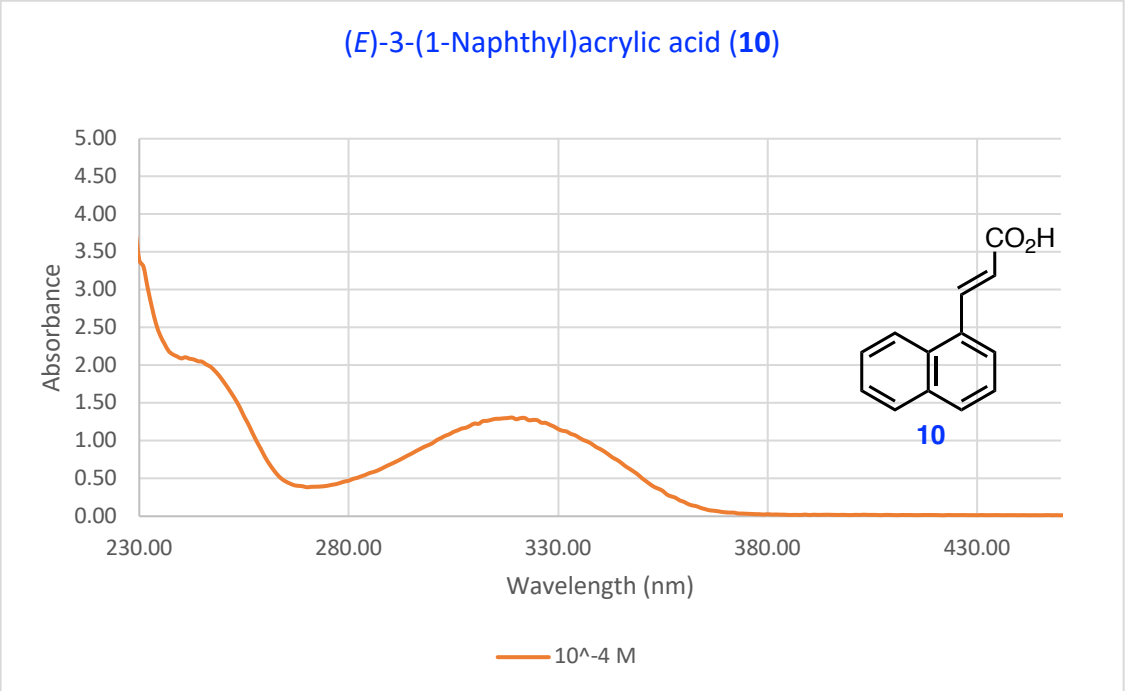


Figure S14. UV-vis absorption spectrum of compound **10** in MeOH (1×10^{-4} M; $\lambda_{max} = 322$ nm, absorption tail up to ca. 390 nm); ε (322 nm) = 1.30×10^4 M^{-1} cm^{-1}.

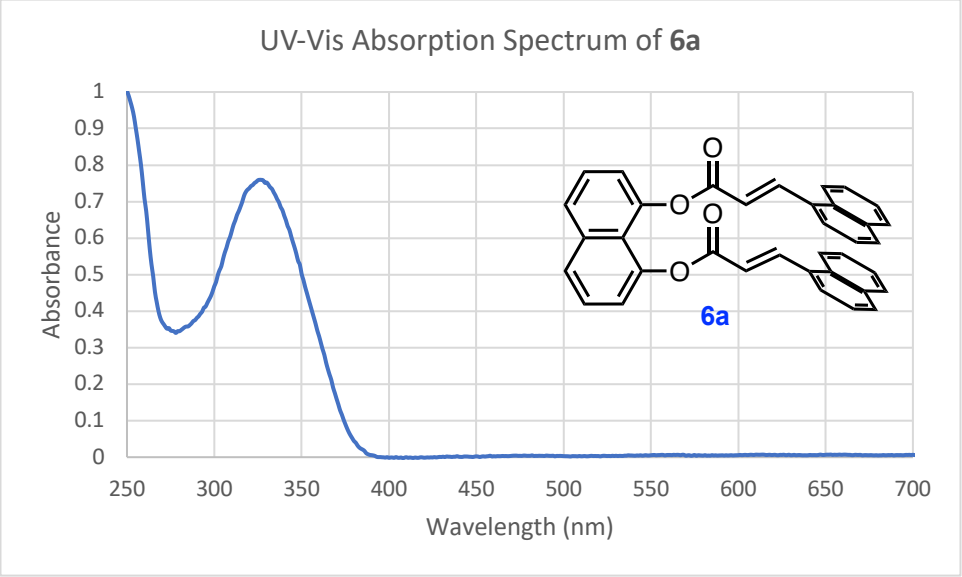


Figure S15. UV-vis absorption spectrum of compound **6a** in CH_2Cl_2 (2.5×10^{-5} M; λ_{max} = 326 nm, absorption tail up to ca. 400 nm); ε (326 nm) = 3.04×10^4 M^{-1} cm^{-1}.

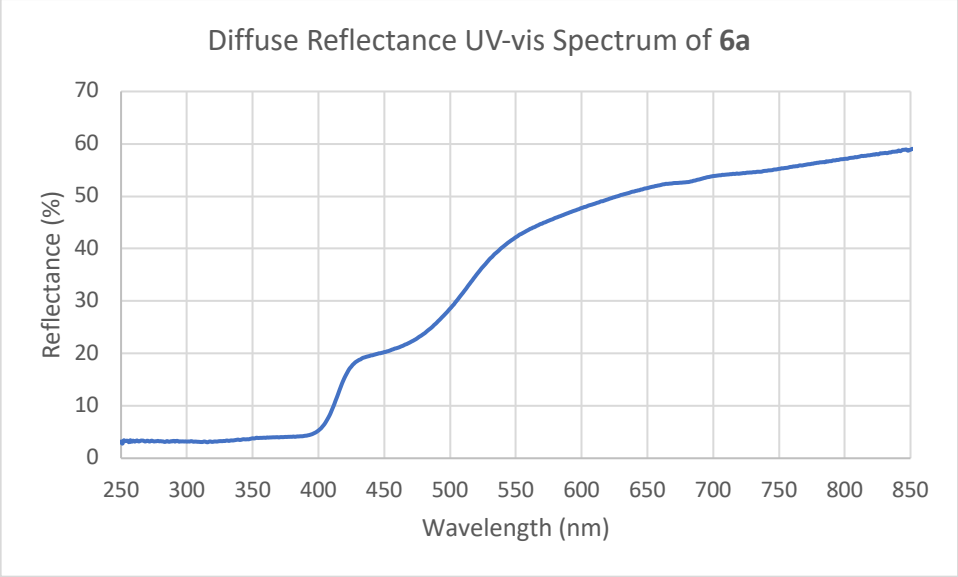


Figure S16. Diffuse reflectance UV-vis spectrum of **6a** in solid powder form.

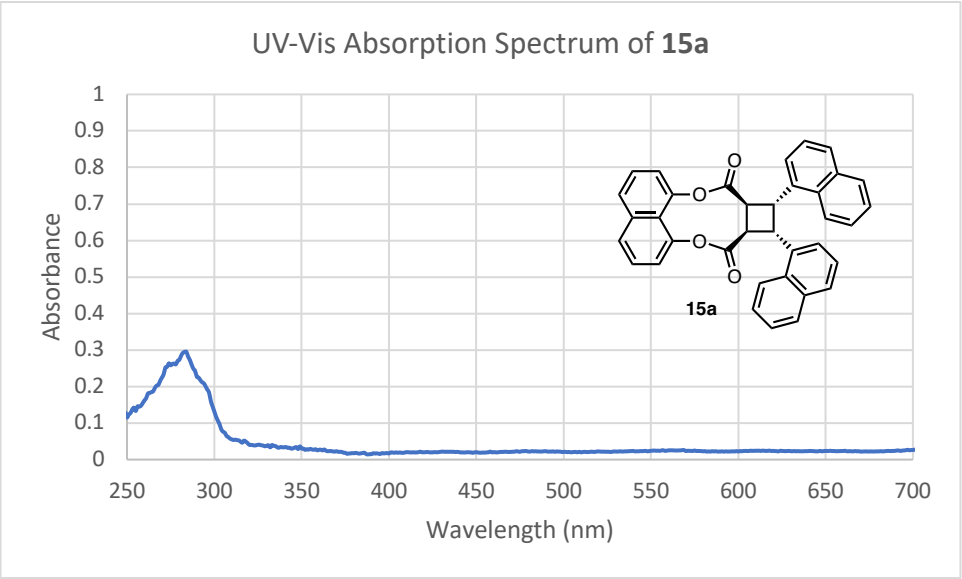
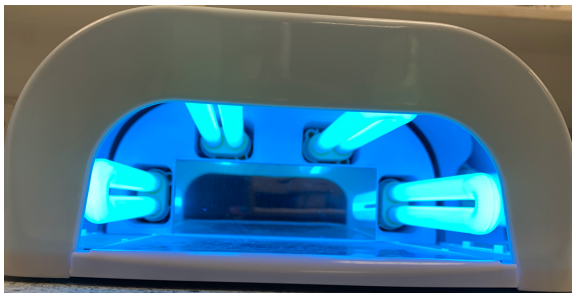


Figure S17. UV-vis absorption spectrum of compound **15a** in CH_2Cl_2 (5×10^{-5} M; λ_{max} = 284 nm); ε (284 nm) = 5.90×10^3 M^{-1} cm^{-1}.

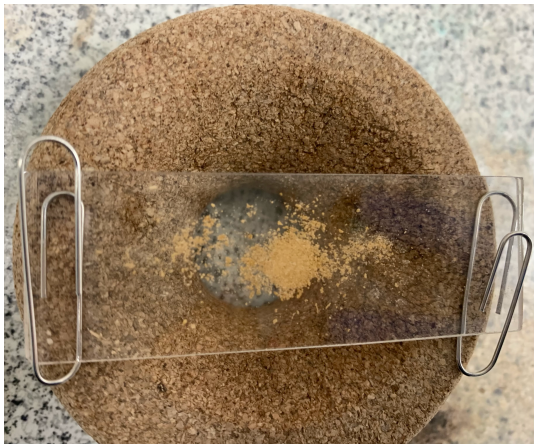
Experimental Set-up for the Photochemical [2+2] Cycloadditions:

a)

b)



c)



d)

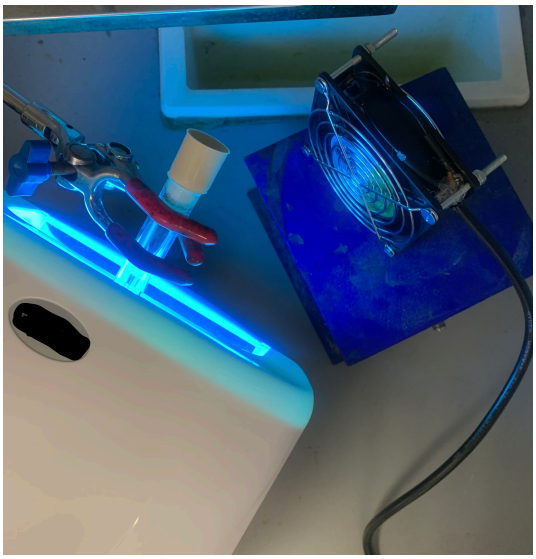


Figure S18. (a) Appearance of the UV gel nail dryer (Beurer, MP38) when it is off. b) Appearance of the UV gel nail dryer with the fluorescent lamps on. (c) Appearance of a powder sample, which was prepared for irradiation and placed between two quartz microscope slides. (d) Irradiation of a solution sample in a quartz test tube inside a fume hood with a cooling fan on.

Four Philips PL-S 9-Watt UV-A fluorescent bulbs were used for irradiation. The emission spectrum of these fluorescent lamps can be accessed via the following link: https://www.lighting.philips.com/prof/special-lamps/insect-trap/actinic-bl/actinic-bl-pl-s-pl-l/927901721008_EU/product (Last accessed on May 23, 2025).

Computational Data

XYZ coordinates:

anti-cis-anti conformer (**15a-*anti-cis-anti*; A**)

There is no negative frequency (imaginary mode) as expected

C	2.74313610998885	0.85289097870194	2.11079569313839
H	1.91632277304693	1.47841954783772	1.77641806958660
C	3.48332359549148	1.25245956526958	3.20493955533392
H	3.22797229304256	2.18045491695847	3.72258013557340
C	4.56535917613499	0.46450254092675	3.66581724628095
H	5.14074065781069	0.78702811323466	4.53750127923536
C	4.89435533539861	-0.70239075339039	3.00759830726919
H	5.73528214283997	-1.31345869520457	3.34731501991428
C	4.15357089669570	-1.13719586487073	1.87380234972686
C	4.49741721166692	-2.33243055538137	1.18202366914757
H	5.34869307503274	-2.92070853799135	1.53523027034355
C	3.76968836450674	-2.73090183572857	0.08488770728083
H	4.03777737954978	-3.64253836230445	-0.45530986865426
C	2.65105899624126	-1.97401561127609	-0.34575586278947
H	2.08358626275963	-2.34034614392045	-1.20202215619925
C	2.26435123341723	-0.81477732457466	0.29987509884816
C	3.04034449641397	-0.35366593652669	1.41861064941333
C	1.02400420672267	-0.05283658639907	-0.08087544280442
H	1.27251232270206	1.00022079886751	-0.27511846616861
C	0.12923489265112	-0.57930333771066	-1.22247159399638
H	0.32604855817961	-1.59828166452021	-1.57124355634318
C	-0.04803358314053	0.33741350486986	-2.40206273951907
C	-1.35864405224307	0.49320296538340	-4.34764287538566
C	-0.79590843472756	0.68876539429921	-5.58676643853988
H	0.17692079298893	0.24086796121152	-5.79826631148869
C	-1.46910036339222	1.46522904185706	-6.55925914405107
H	-1.01143574767849	1.61017227253192	-7.54053531565085
C	-2.68292142003914	2.04325957315046	-6.26160039294723
H	-3.20427036503502	2.65564248695312	-7.00125267590384
C	-3.28974082013739	1.85659144541053	-4.98802927211459

C	-4.54317917560603	2.45591377107640	-4.68087116870166
H	-5.02598359901171	3.07127222912241	-5.44384885103982
C	-5.13964868267532	2.26439006634567	-3.45421688779562
H	-6.10221812294485	2.72887408153351	-3.22796323297226
C	-4.51757505595922	1.44979380419472	-2.47906458038505
H	-4.99386959866124	1.26905554480622	-1.51463985374712
C	-3.30458918805102	0.86038242686080	-2.75187814324729
C	-2.62955242817846	1.04959698995155	-3.99801179391105
C	-2.16453711153769	0.44555869620405	-0.67308088511838
C	-1.11371867843278	-0.54782474990337	-0.24498191954754
H	-1.58304745005110	-1.53620512758751	-0.14813292855940
C	-0.21138414223921	-0.10795118014718	0.92656077797073
H	-0.48696163997012	0.90045246906079	1.24595516134942
C	-0.07803712572735	-1.03689461353760	2.10283262302461
C	0.05737786950478	-2.39982147272799	1.88839125907193
H	-0.01320919233580	-2.79935809249263	0.87473188772309
C	0.32127409053637	-3.30247166926792	2.94344890732097
H	0.42945144106241	-4.36785189640944	2.72474031612501
C	0.45793424625726	-2.83638560735938	4.23199764899268
H	0.67959929059665	-3.52057295839514	5.05558405080082
C	0.30628284040683	-1.45199455840258	4.51417753047813
C	0.43904002446825	-0.96096021443327	5.84408695772819
H	0.66764891206810	-1.67436861003873	6.64081454204322
C	0.28061640082526	0.37803119175255	6.12723356915301
H	0.38478487355901	0.74250086137165	7.15248832187267
C	-0.02807072792692	1.28450193172859	5.08257839109543
H	-0.16648560869937	2.34511653415371	5.30826228826201
C	-0.15364525374676	0.84057082851998	3.78312289038003
H	-0.38962339373784	1.56546638099074	3.00423083612097
C	0.01681445794756	-0.53366103969419	3.44546963672205
O	0.20494644856561	1.51617980059438	-2.41820652507750
O	-0.67042846733242	-0.29833231954771	-3.42956696332204
O	-2.71866647216563	-0.00216370584865	-1.83617943604983
O	-2.43628081933057	1.49505854060074	-0.15552931774297

Transition state-1 (**16a**; **B**)

only one imaginary mode exists since it is the TS

C	2.62180765395658	0.76432802726734	1.90058281232112
H	1.74639976562316	1.33952428737988	1.60458511280134
C	3.32505559837877	1.15106411351438	3.02168798714641
H	2.98589113209669	2.01187941355291	3.60292951472961
C	4.47740212323213	0.43643086095467	3.42546009827248
H	5.02457044071639	0.74651740118406	4.31936594495244
C	4.91206843700285	-0.64029953298595	2.68289178673202
H	5.81118886861069	-1.18914435807389	2.97665741952016
C	4.21027861124065	-1.06084630185590	1.52038508621116
C	4.66736577783142	-2.15487187459693	0.73555352878329
H	5.57746557762048	-2.67855169379208	1.04048323260557
C	3.98100955815598	-2.53516731048077	-0.39380671290145
H	4.34431805885742	-3.36138982167297	-1.01010279015744
C	2.78777920716940	-1.86755507044625	-0.76242577405277
H	2.26847348429116	-2.18579877978738	-1.66822799272894
C	2.28674399312601	-0.81641230742085	-0.01682223577434
C	3.02168571703185	-0.35978333052945	1.12740422767334
C	0.98432048871970	-0.15772809550513	-0.38677187308175
H	1.17409545618766	0.86109360573794	-0.76439357143150
C	0.02236755245492	-0.89858255308463	-1.35643213664119
H	0.17567793584946	-1.98420636202397	-1.28756389293670
C	0.07436490720621	-0.53576520290399	-2.82498150168129
C	-1.57121141830698	0.78014840141161	-4.18854808193395
C	-0.93041928395656	0.93285989662272	-5.39742752668079
H	0.07099886159481	0.52569353313719	-5.53101386374690
C	-1.59817869820438	1.63110967874707	-6.43261368354162
H	-1.09657899981203	1.75838783250091	-7.39490429568683
C	-2.85583368285548	2.15624637016844	-6.23327373938914
H	-3.35903994147206	2.70435725757112	-7.03346861876598
C	-3.53374324816049	1.99640193031153	-4.99099615842002

C	-4.83690304387155	2.52378486211359	-4.78046113749241
H	-5.31634181764029	3.07629169700721	-5.59212739913334
C	-5.48460238600165	2.33821074954949	-3.57945610142962
H	-6.48589417073488	2.74691329781306	-3.42411900653595
C	-4.86573013361356	1.61013307893554	-2.53727328248111
H	-5.37721352292721	1.43905319110868	-1.58859990956958
C	-3.60389381889581	1.08588955926852	-2.70530657083847
C	-2.88776852336754	1.27662022731172	-3.93350609527018
C	-2.00131647163651	0.69317453207404	-0.99121704422373
C	-1.19611754148362	-0.47993728390811	-0.46005052428210
H	-1.87390597030864	-1.31112416273252	-0.22310969630718
C	-0.19986457606306	-0.05896525322771	0.65909257850206
H	-0.37692645436356	0.98146381582415	0.93781679092192
C	-0.12096817290286	-0.94229142868301	1.87613203479351
C	0.12103186571285	-2.29905023804286	1.73522159043161
H	0.21465481189296	-2.73310609211362	0.73874049512258
C	0.28717101766719	-3.15193332620117	2.84832098098844
H	0.48598658769340	-4.21413749590000	2.68633701269592
C	0.21692234141996	-2.64103654967545	4.12366343856575
H	0.36041879566187	-3.28693758240253	4.99397516713268
C	-0.04439264343048	-1.26114822432733	4.33084588220645
C	-0.11809818128324	-0.72347670393472	5.64586729082144
H	0.03479399283807	-1.39866044589278	6.49237031000652
C	-0.37536556166004	0.61228365986832	5.85656094764864
H	-0.42758826131409	1.01201442708367	6.87242562221493
C	-0.58113753251643	1.46871379277388	4.74798696921851
H	-0.79947258193894	2.52697166524721	4.91324840303580
C	-0.51359775680947	0.97855391644929	3.46138476441132
H	-0.68745000489531	1.66547334506393	2.63314780702617
C	-0.23302829572140	-0.39392802445346	3.19963355110972
O	0.93520747514954	-0.82546867742934	-3.61273967953574
O	-1.02541764371714	0.18816551703133	-3.08703146431518
O	-3.09803427987168	0.27572171758999	-1.69525757414477
O	-1.73148147525332	1.85182842190942	-0.82672845349095

anti-cis-syn conformer (**15a-*anti-cis-syn***; **C**)

There is no negative frequency (imaginary mode) as expected

C	2.62087533057121	0.95956921140150	1.69092977556326
H	1.72544040656254	1.46630400408546	1.33342512991506
C	3.41302188731632	1.58486363752250	2.63228130416726
H	3.13019912729211	2.57017563618411	3.01127762703926
C	4.58555039462165	0.95556291646563	3.11544316919610
H	5.20236332179949	1.45670630431844	3.86600252525836
C	4.94974789902515	-0.28358514056524	2.63062959400821
H	5.85952811439845	-0.77454638885943	2.98732708780971
C	4.15723243248843	-0.94994984965245	1.65532671813469
C	4.53800461293271	-2.21933191764817	1.13665577339314
H	5.45778571283944	-2.68427424286485	1.50184569669228
C	3.76063372631284	-2.84099303013938	0.18709553573993
H	4.05611028823570	-3.81051729767746	-0.22207890665533
C	2.55751721469275	-2.23877445008314	-0.25973688697148
H	1.95817598405811	-2.77385838482866	-0.99767533376028
C	2.13419421773011	-1.01488504847515	0.22337260856471
C	2.95411801419647	-0.32635873672798	1.18204082269367
C	0.82291499609621	-0.39927260446786	-0.18103432531132
H	0.99327526497784	0.61363871645152	-0.57193004306181
C	-0.12043277593869	-1.17128233451380	-1.14304589496331
H	0.06326378393115	-2.24903694856304	-1.18367440219041
C	-0.27541501357699	-0.67933715301881	-2.55599978153487
C	-1.07735624684860	1.30503890609734	-3.62385075202655
C	-0.30540074795681	1.99794538927304	-4.52634203638866
H	0.78067316681264	1.97096927525085	-4.41994958519257
C	-0.92134894239091	2.74388806135683	-5.55871181025572
H	-0.29831709237618	3.29016905627868	-6.27061594588869
C	-2.29469624535632	2.78807975977438	-5.65441002849939
H	-2.77920273774437	3.37126272843545	-6.44127132673567
C	-3.11644477864668	2.07956785019511	-4.73379088490457

C	-4.53525966794045	2.13005029696297	-4.83008854214522
H	-4.98135296545396	2.73018588738152	-5.62676883947424
C	-5.33079198340762	1.43856556289471	-3.94356312095529
H	-6.41930181353301	1.48340566825395	-4.02423303151638
C	-4.74171878714090	0.65239046717380	-2.92534749112636
H	-5.35581848683100	0.07802480540157	-2.22918095670468
C	-3.37302606746213	0.58631230698215	-2.81119413934498
C	-2.50428387346615	1.30100181453694	-3.69193360767001
C	-2.26265184394734	0.19506563036273	-0.73457454725202
C	-1.31766624191632	-0.84333092905058	-0.18149766783866
H	-1.90675530426456	-1.73388190393619	0.08334811247501
C	-0.34434887608782	-0.31786994629876	0.89764326293973
H	-0.58001569439199	0.71714865036674	1.15667583113497
C	-0.15748428110792	-1.15930965899506	2.13229562311462
C	-0.07949367300441	-2.53913284357409	2.02141744989859
H	-0.21837640179151	-3.01528937578613	1.04875367587300
C	0.20243504623716	-3.36697367443203	3.13182776431501
H	0.26013936618917	-4.44958017197830	2.99331742148144
C	0.41519488895723	-2.80877524331987	4.37236428624272
H	0.64741457344187	-3.43601279189493	5.23728636191348
C	0.33042213983952	-1.40159945381386	4.54974548949663
C	0.54057529318303	-0.81587265161080	5.83054445157988
H	0.77609407472553	-1.47504221430025	6.67078997100924
C	0.44675740101506	0.54626230196395	6.01398487778870
H	0.60969550065721	0.98359308835983	7.00242285131475
C	0.12928619593237	1.38191607730005	4.91454855971316
H	0.04438183967683	2.46184712735705	5.06113757863485
C	-0.07186312490361	0.84530505869249	3.66029666380794
H	-0.31237016969560	1.51832072970321	2.83804686623464
C	0.02753382183095	-0.55718115818424	3.42460314730002
O	-0.30544758389004	-1.34486108861456	-3.55555713763633
O	-0.44820156627474	0.67802036948283	-2.55529002142184
O	-2.83027191002226	-0.28992084705620	-1.87679776945350
O	-2.48873619284272	1.28964841540353	-0.29484075001046

Transition state-2 (**16b**; **D**)

only one imaginary mode exists since it is the TS

C	2.70840268566389	0.71476444422736	1.41509988866989
H	2.00234954021201	1.32905643329924	0.85945672742008
C	3.36512804513116	1.27148960329620	2.49346189195871
H	3.16000321413911	2.30693589094597	2.77549135520869
C	4.28957390713634	0.50645499752841	3.24401964258287
H	4.79782038510373	0.95325462524816	4.10249839198902
C	4.55406138222188	-0.79695236939081	2.88041814873365
H	5.27778823906296	-1.39470659559961	3.44158306195990
C	3.89677669943930	-1.39635064736145	1.77026660176942
C	4.17457271058243	-2.73906054385330	1.39209532509998
H	4.91247055394201	-3.30733408254442	1.96483629316427
C	3.52234050464925	-3.30572116708515	0.32222031392448
H	3.73835413657179	-4.33482062165497	0.02369444963731
C	2.54302330392924	-2.57001931319581	-0.38966330127145
H	2.01879106749521	-3.07468032053883	-1.20196190674422
C	2.22395980904406	-1.26557815053815	-0.05791051153089
C	2.93301856766219	-0.63522897385368	1.02491933550401
C	1.06854581724295	-0.53430962430394	-0.69722727656830
H	1.31889207807621	0.51898273933493	-0.86817109966272
C	0.39437468131492	-1.19957859243858	-1.92583981836483
H	0.94690553442497	-2.00835072552353	-2.41596424289650
C	-0.04100926629414	-0.27279907685682	-3.04485928516590
C	-1.19405721725966	1.78155364423558	-3.36278022493630
C	-0.70780907560568	2.91625407760900	-3.97194996365452
H	0.36251753936424	3.12322634740333	-3.91564391168593
C	-1.58486373509837	3.79783717060505	-4.64746147502476
H	-1.17916714718068	4.69411557445856	-5.12274418303684
C	-2.93547009761342	3.53080493606385	-4.70255622511958
H	-3.61788596854048	4.21026167316023	-5.21888118147213
C	-3.47155449447117	2.36825384838431	-4.08235230587401

C	-4.86737010481187	2.08306001870213	-4.11549350609068
H	-5.52689348937237	2.77869937008915	-4.63983106416380
C	-5.38033801187311	0.95943171295350	-3.50444483411460
H	-6.45322712317795	0.75584961998695	-3.54045140124111
C	-4.53081021484707	0.04694053571316	-2.83062017516653
H	-4.92316630156846	-0.85105675546270	-2.35512694465427
C	-3.18019523529219	0.31008299301339	-2.79272249755962
C	-2.59226370796184	1.46449688696103	-3.40072445399997
C	-2.20958899696008	-1.55986251930130	-1.39813505601936
C	-0.76221256670778	-1.72264521027825	-0.98810383820839
H	-0.58219267409070	-2.76712457937743	-0.71001077637177
C	-0.29683625177943	-0.70943429048944	0.09904385356427
H	-0.87282892284226	0.21278519256386	-0.03360484020835
C	-0.24405651496067	-1.09713481780601	1.54867178049810
C	-0.05112952622299	-2.41459958657763	1.92559324074799
H	-0.04051986061554	-3.20029699045793	1.16923795594996
C	0.17230945211614	-2.78042589622079	3.27375084525759
H	0.32495600785366	-3.83288361499961	3.52582313530237
C	0.22170337507840	-1.81495428358223	4.25330237090138
H	0.42137079684083	-2.08247279967463	5.29443548698906
C	0.01211505107856	-0.44787098939698	3.92558398708405
C	0.07249746049417	0.56165118667225	4.92649447911244
H	0.28441845024745	0.26216456188472	5.95667700353883
C	-0.13028381534376	1.88811723947955	4.61177122694180
H	-0.07803140833502	2.65441588227309	5.38952297942080
C	-0.41621929819523	2.25710865870401	3.27422119494514
H	-0.58913398280478	3.30766411613603	3.02639003648237
C	-0.47174573095906	1.30176448115999	2.28035391344435
H	-0.68151167394083	1.62262137879867	1.25968666489647
C	-0.24949928298426	-0.07677305366257	2.56249129284943
O	-0.15611811244269	-0.61657302857992	-4.19310935218275
O	-0.29529280685331	1.00568365809602	-2.63155801098026
O	-2.23980342783156	-0.48696667807659	-2.21026580462776
O	-3.16595495128067	-2.19921760030458	-1.04294340695058

syn-cis-syn conformer-2 (**15a-*syn-cis-syn;* E**)

There is no negative frequency (imaginary mode) as expected

C	2.85035288355691	0.61501281601431	1.67938983295660
H	2.16551985928379	1.23065254655734	1.09864667214458
C	3.45181348144906	1.16348335417305	2.79361482623355
H	3.23157984180210	2.19633578533101	3.07483179605512
C	4.34379912211180	0.39499012851369	3.57924355355917
H	4.80938599628648	0.83641584123729	4.46427833685016
C	4.62740240936629	-0.90565501174944	3.21902539489900
H	5.32213051054752	-1.50762425833865	3.81144667431423
C	4.02599802911785	-1.49674282851824	2.07332850286936
C	4.32033014469287	-2.83759423842675	1.70020740496319
H	5.02669230209636	-3.41146560951864	2.30615622771514
C	3.72268423065857	-3.39479563578927	0.59407132357171
H	3.95005982972896	-4.42287082142545	0.30065469410648
C	2.78724188242551	-2.64941445922554	-0.16581970957126
H	2.30849628065820	-3.14688594147664	-1.00992637882260
C	2.45730873109417	-1.34611108045912	0.15683310576963
C	3.10298268806620	-0.72883216708213	1.28557131809583
C	1.35267244140473	-0.59203612857686	-0.53919758840396
H	1.64905169744773	0.45102661408470	-0.70813425284531
C	0.72282228867417	-1.24892324399192	-1.80411883039409
H	1.25587505706410	-2.10205960584881	-2.23344490760497
C	0.41853590384168	-0.30518915124053	-2.93989737466057
C	-1.21446626559841	1.43215415944583	-3.33051008519531
C	-0.69143858837769	2.22287617069517	-4.32873758531330
H	0.38890407589074	2.26316801927419	-4.46794333590355
C	-1.55567571930220	2.97739928297276	-5.15583764490668
H	-1.13014793657273	3.59965241612259	-5.94651790845809
C	-2.91794945848540	2.93175333253128	-4.95993381808347
H	-3.59070344359541	3.51688089591027	-5.59154223395353
C	-3.48369597274211	2.12970670065942	-3.92997810070207

C	-4.89127709492444	2.10017790231296	-3.72178267267519
H	-5.52550495353249	2.70660850874680	-4.37286312517868
C	-5.44369482698964	1.33059566528167	-2.72276671792998
H	-6.52490256436647	1.31544857643112	-2.56729775602056
C	-4.61101301151318	0.54577794865266	-1.89093082945425
H	-5.03066495622497	-0.07497900305443	-1.09710233591658
C	-3.24797323574292	0.55363647483043	-2.07127046619265
C	-2.62218013948277	1.34435464876556	-3.08782376872239
C	-1.83473886813323	-1.28526927933380	-1.67698393514798
C	-0.55156079763019	-1.60961676369938	-0.95264007989866
H	-0.54518136135447	-2.68222893133311	-0.72311379118875
C	-0.06101437149694	-0.69871826125478	0.19074898528028
H	-0.56446827996708	0.26578845594266	0.10006866675897
C	-0.07670550545852	-1.17545703076395	1.61519027923111
C	0.07955576035807	-2.51870225742793	1.91320546873801
H	0.11906999117523	-3.25363607991225	1.10809646480630
C	0.23038136240992	-2.97846167208644	3.24224553230187
H	0.35964984547249	-4.04767938113637	3.42829544994636
C	0.23416204100306	-2.08257989914555	4.28743435119722
H	0.37012349787831	-2.42275223121702	5.31762269470898
C	0.05742077164608	-0.69375834683520	4.04217065099654
C	0.06372701838785	0.24372165744263	5.11303233108008
H	0.20832825751417	-0.13000588437248	6.13056882647184
C	-0.10983772960548	1.59093737618964	4.87991202970457
H	-0.10214405037664	2.30088012451378	5.71105962955032
C	-0.30638430116517	2.05503811483054	3.55577777721422
H	-0.45390564066790	3.12245572564779	3.37178968354915
C	-0.30845193625291	1.17149111989667	2.49655746295561
H	-0.45231937019949	1.56259649877236	1.48919391111140
C	-0.12021170042169	-0.22676168949645	2.69458697076650
O	0.75774530482691	-0.43021463013890	-4.08474645475815
O	-0.37954589899065	0.71278814086662	-2.48817840371900
O	-2.46614483596791	-0.18648007746023	-1.18993574400395
O	-2.20863172279882	-1.87182140231053	-2.66198899484756

References

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^{1}H and ^{13}C{^{1}H} NMR spectra:

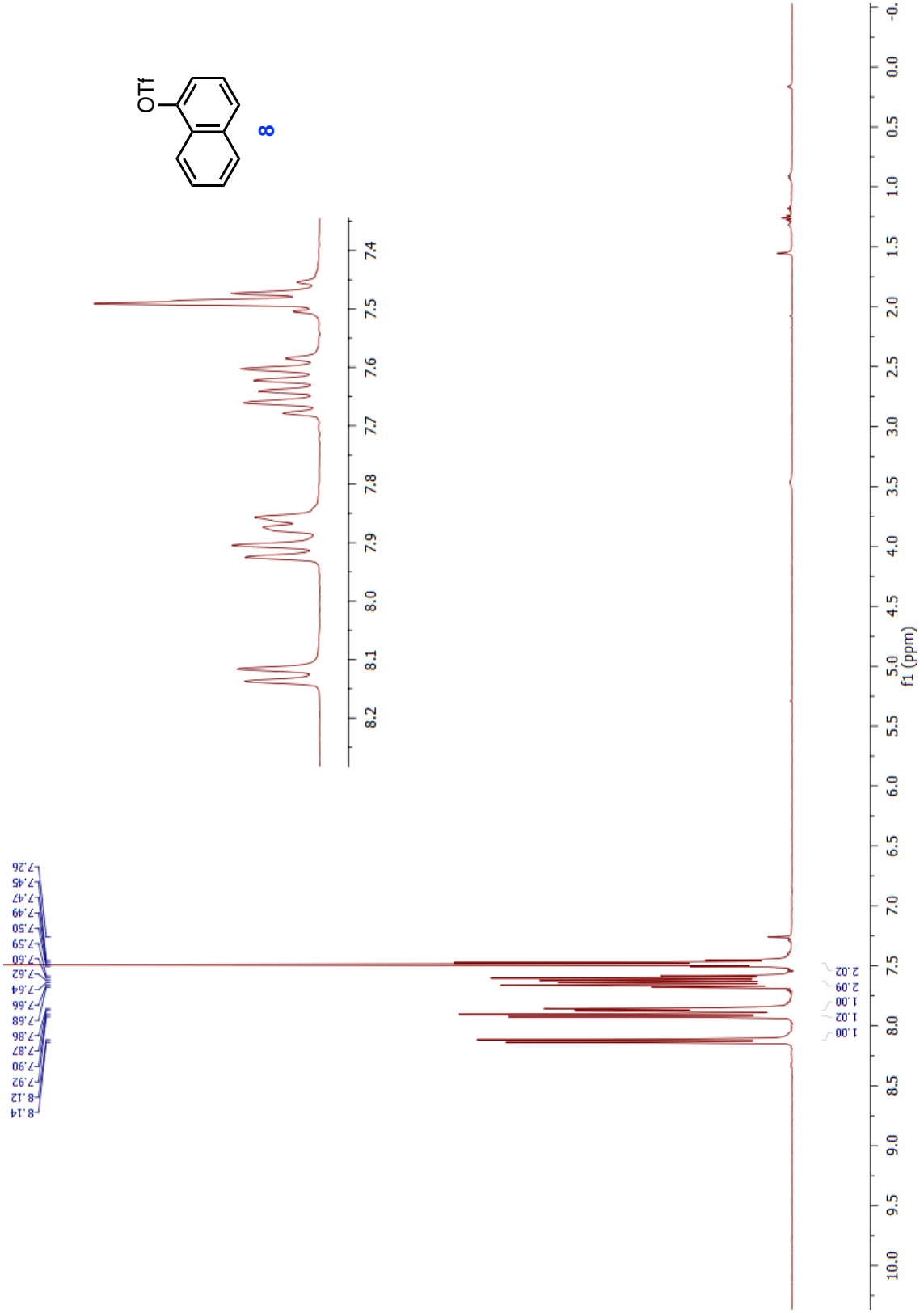


Figure S19. ^{1}H-NMR spectrum of **8** in $CDCl_3$.

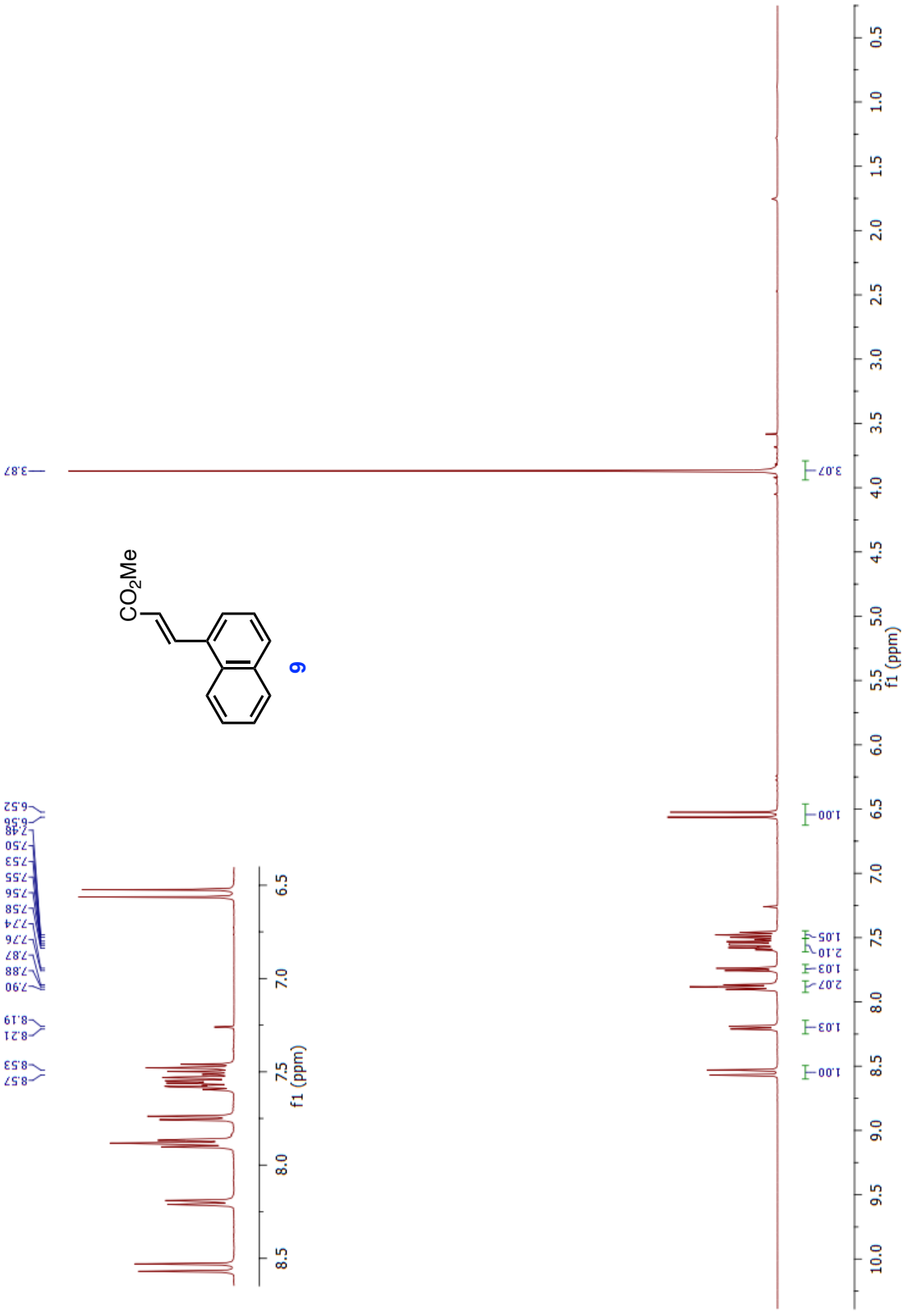


Figure S20. ^{1}H-NMR spectrum of **9** in $CDCl_3$.

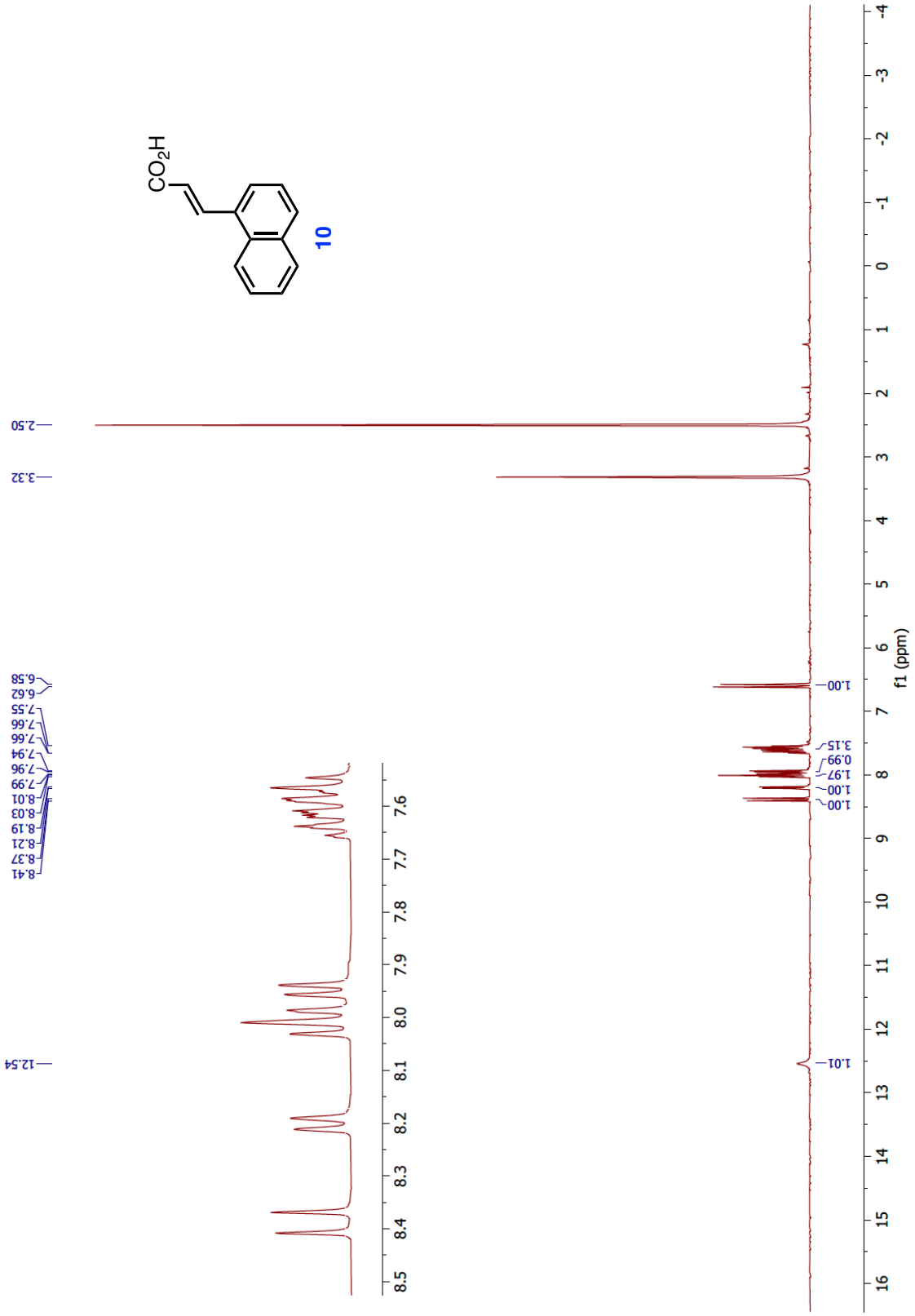


Figure S21. ^{1}H-NMR spectrum of **10** in DMSO-d_6.

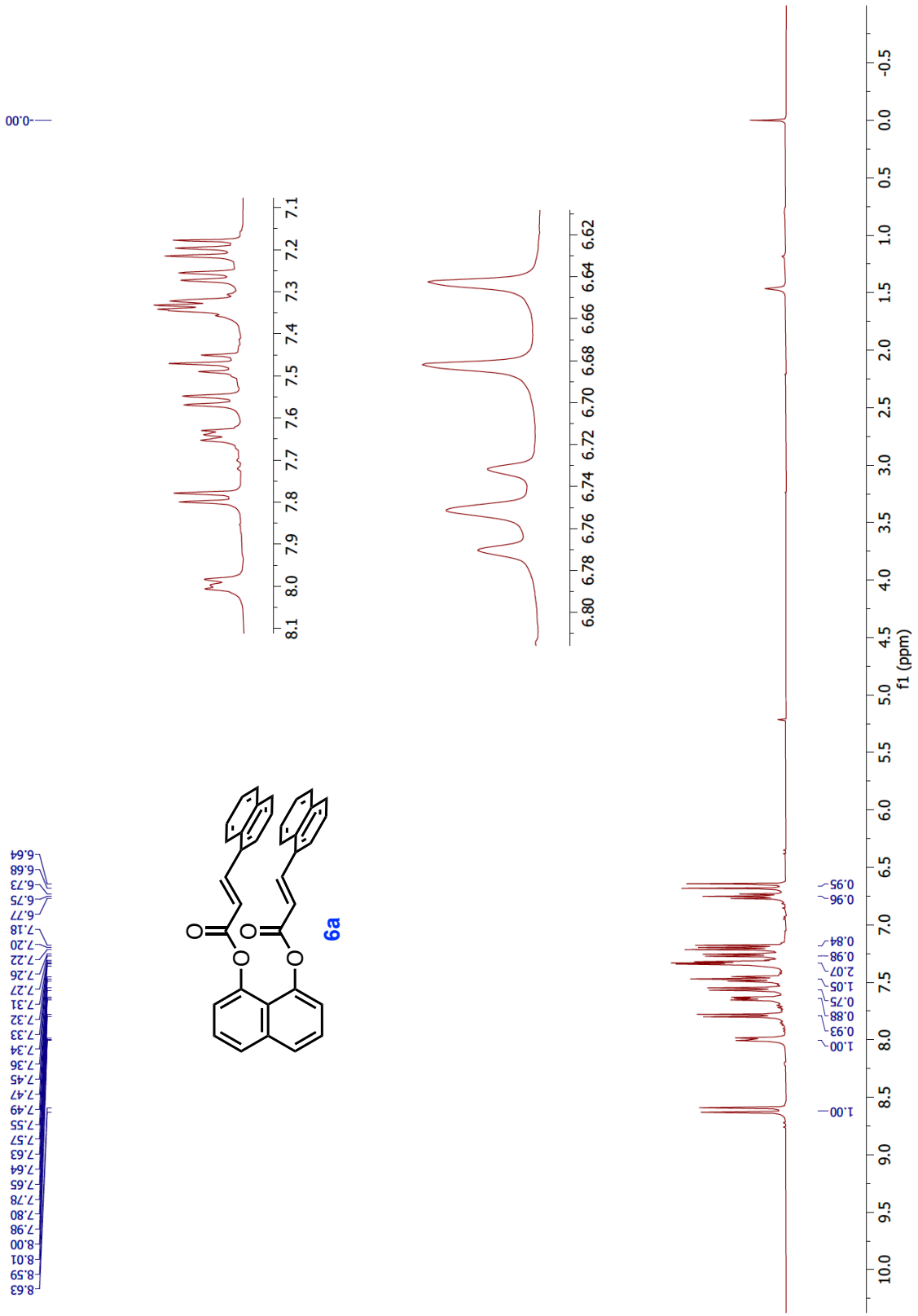


Figure S22. ^{1}H-NMR spectrum of **6a** in $CDCl_3$.

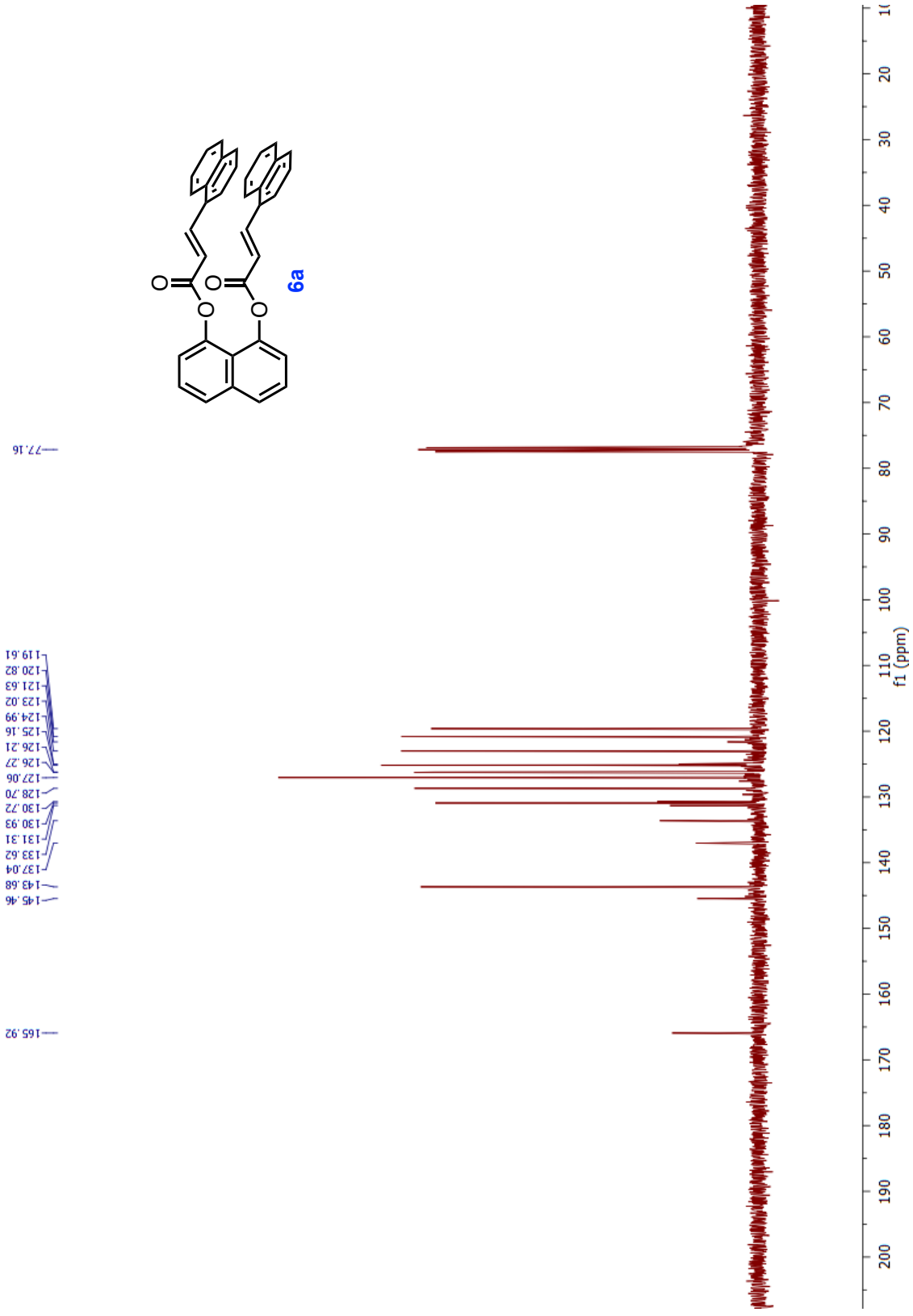


Figure S23. $^{13}C\{^{1}H\}$-NMR spectrum of **6a** in $CDCl_3$.

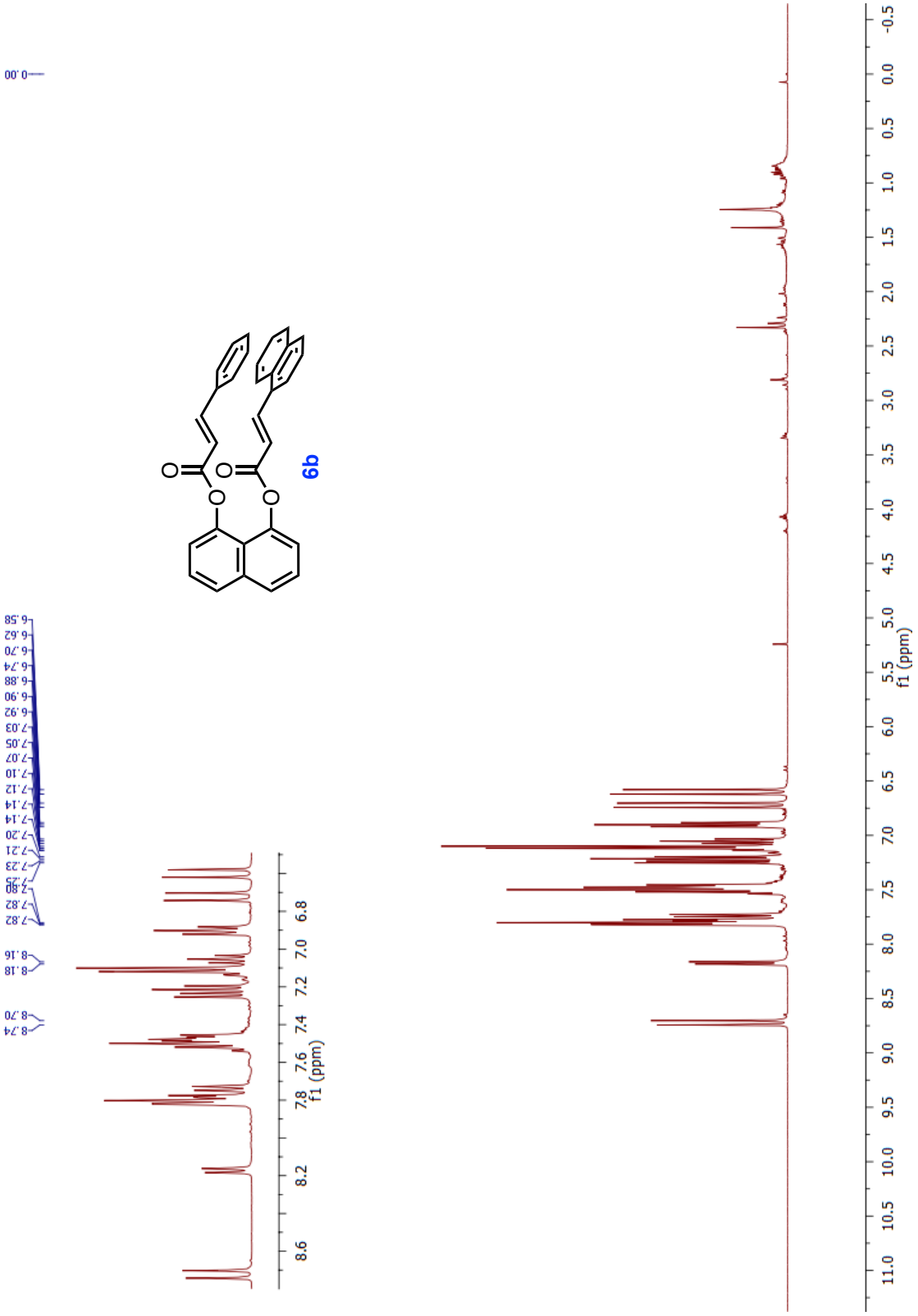


Figure S24. ^{1}H-NMR spectrum of **6b** in $CDCl_3$.

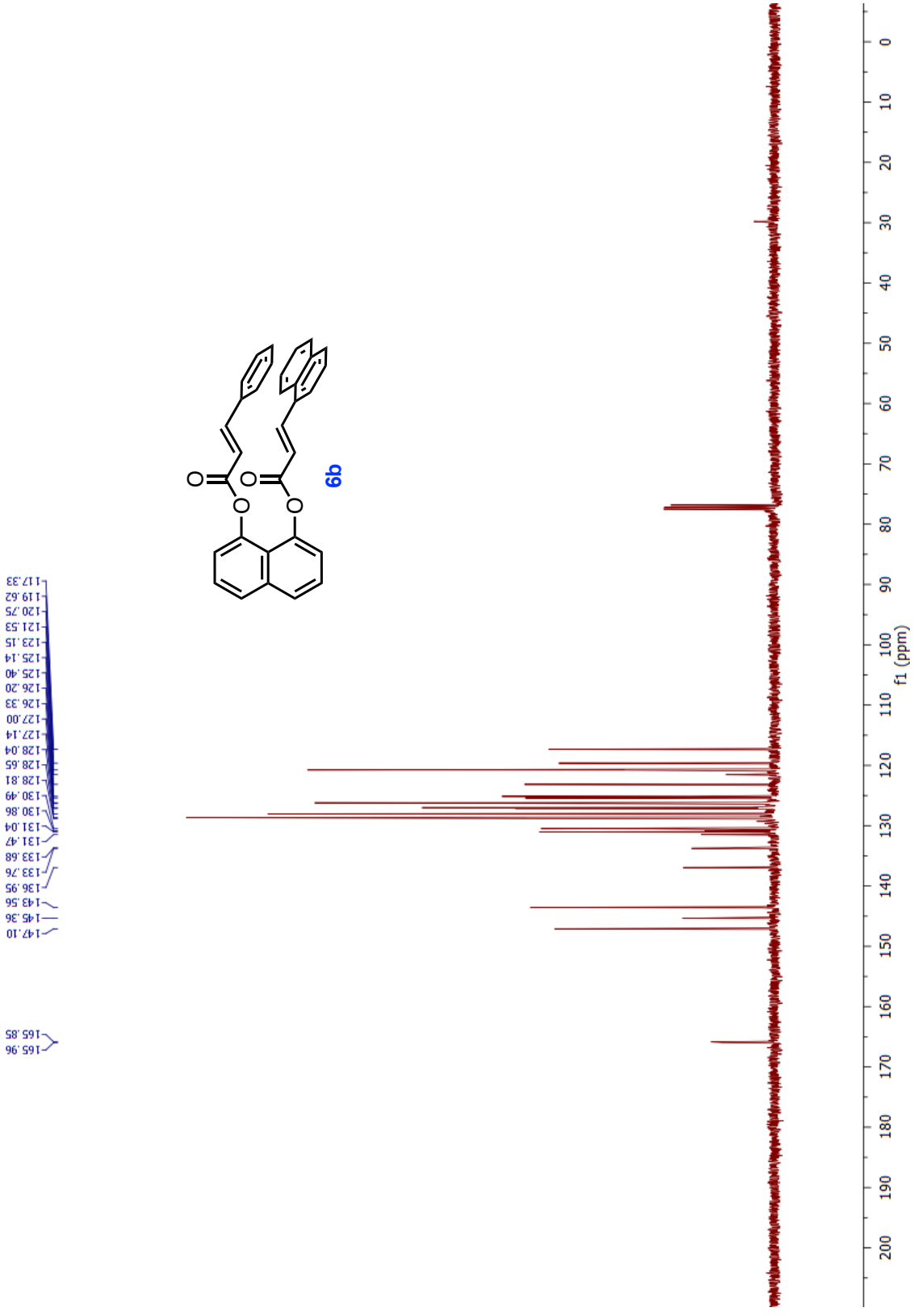


Figure S25. $^{13}C\{^{1}H\}$-NMR spectrum of **6b** in $CDCl_3$.

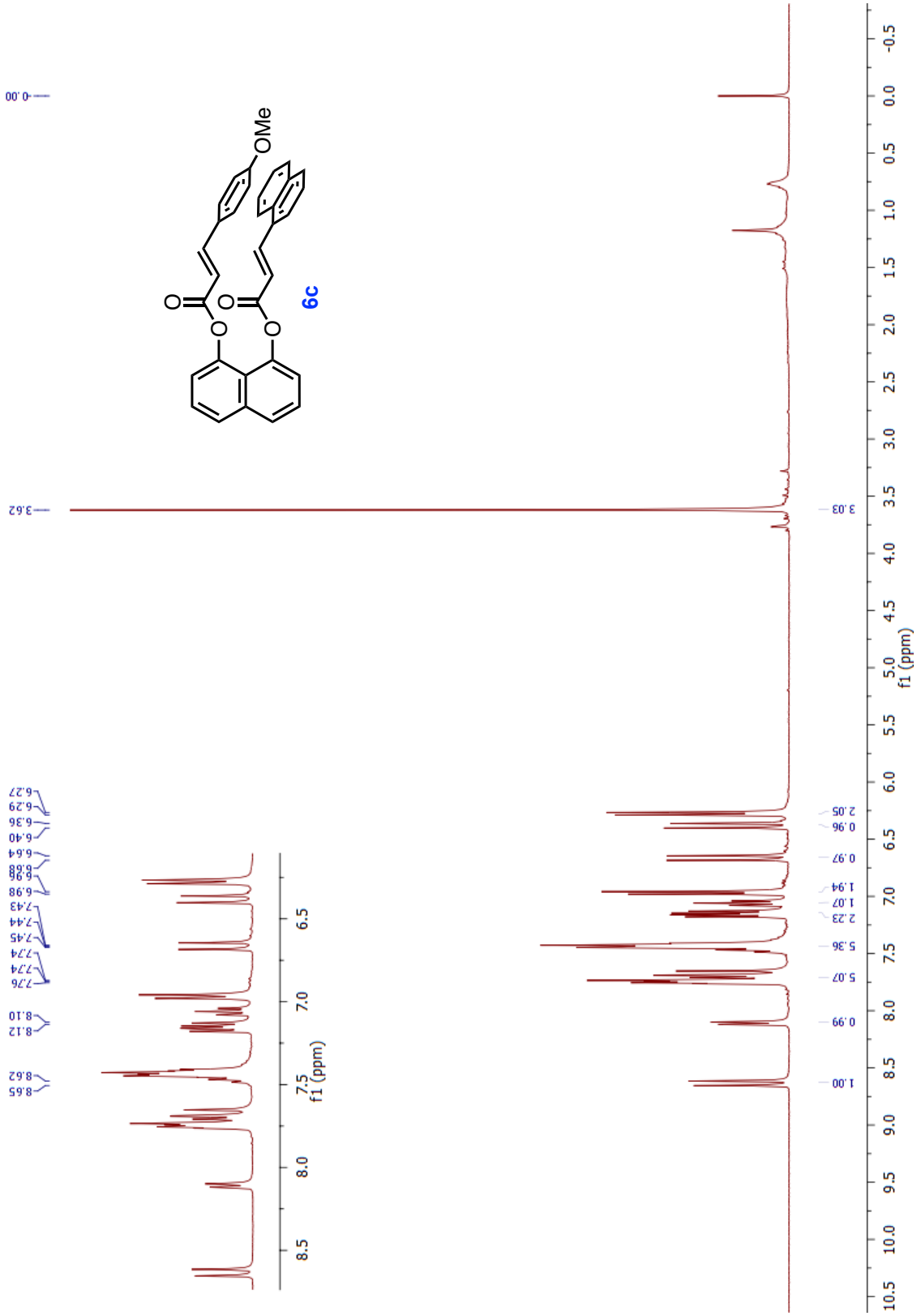


Figure S26. ^{1}H-NMR spectrum of **6c** in $CDCl_3$.

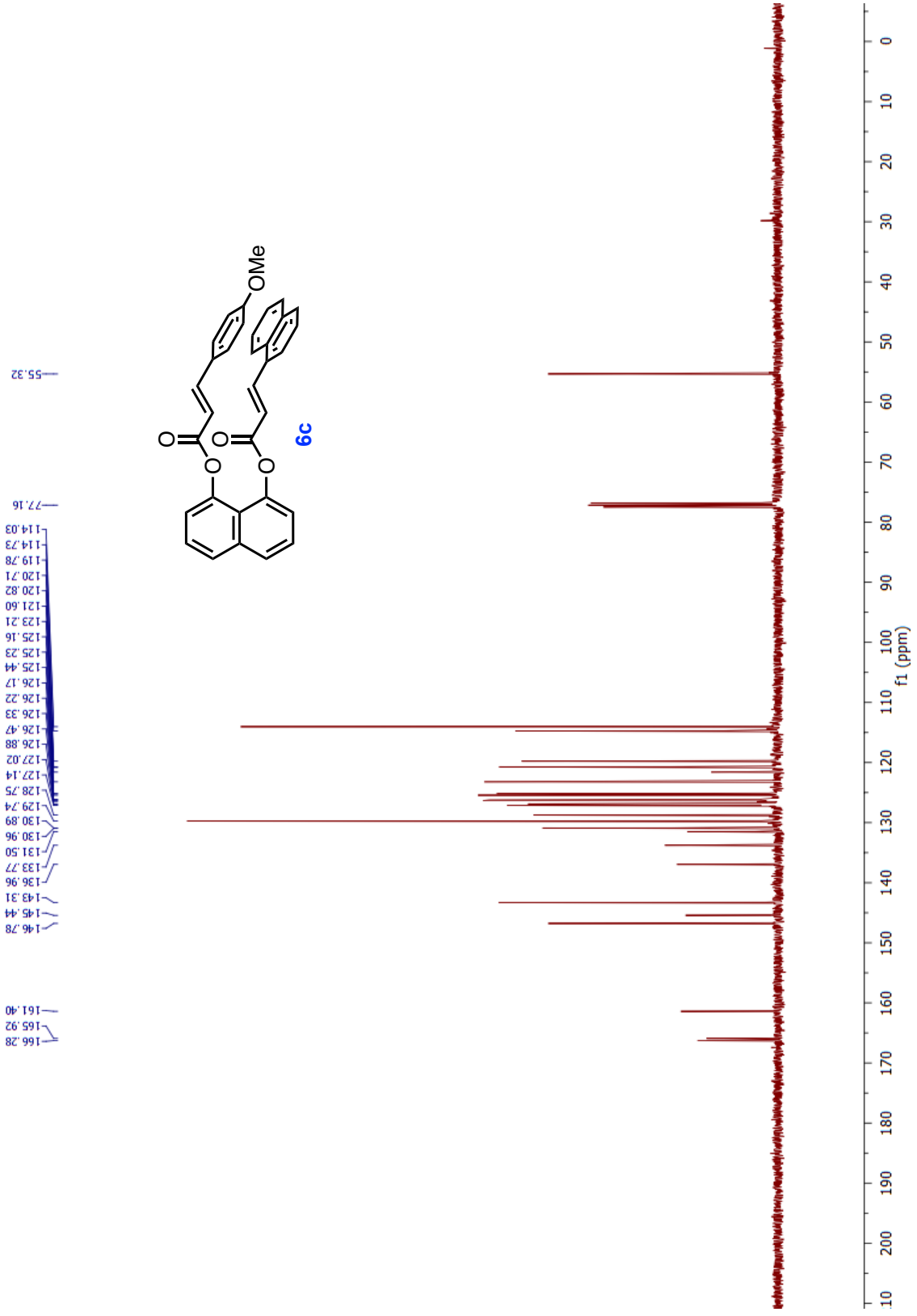


Figure S27. $^{13}C\{^{1}H\}$-NMR spectrum of **6c** in $CDCl_3$.

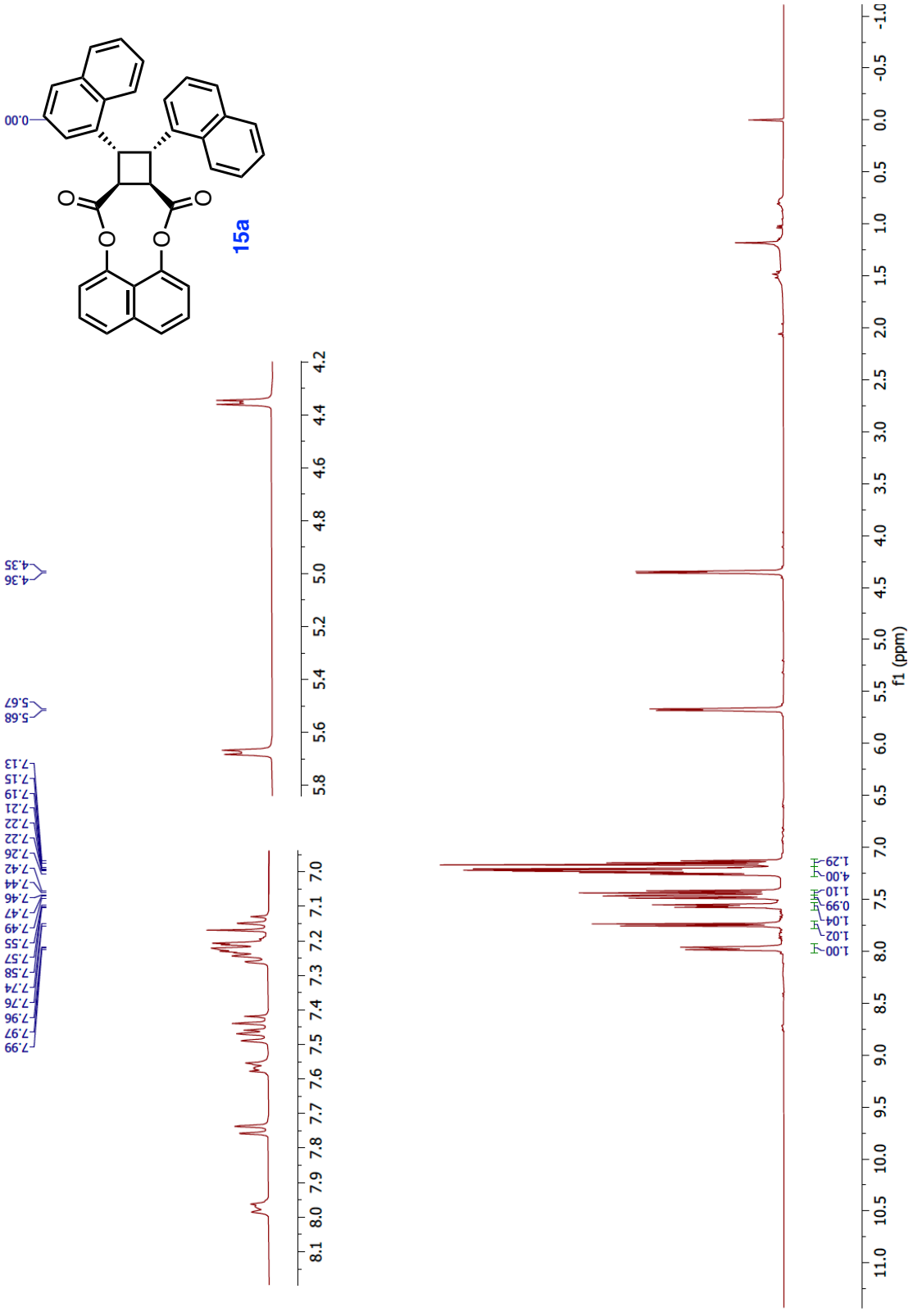


Figure S28. ^{1}H-NMR spectrum of **15a** in $CDCl_3$.

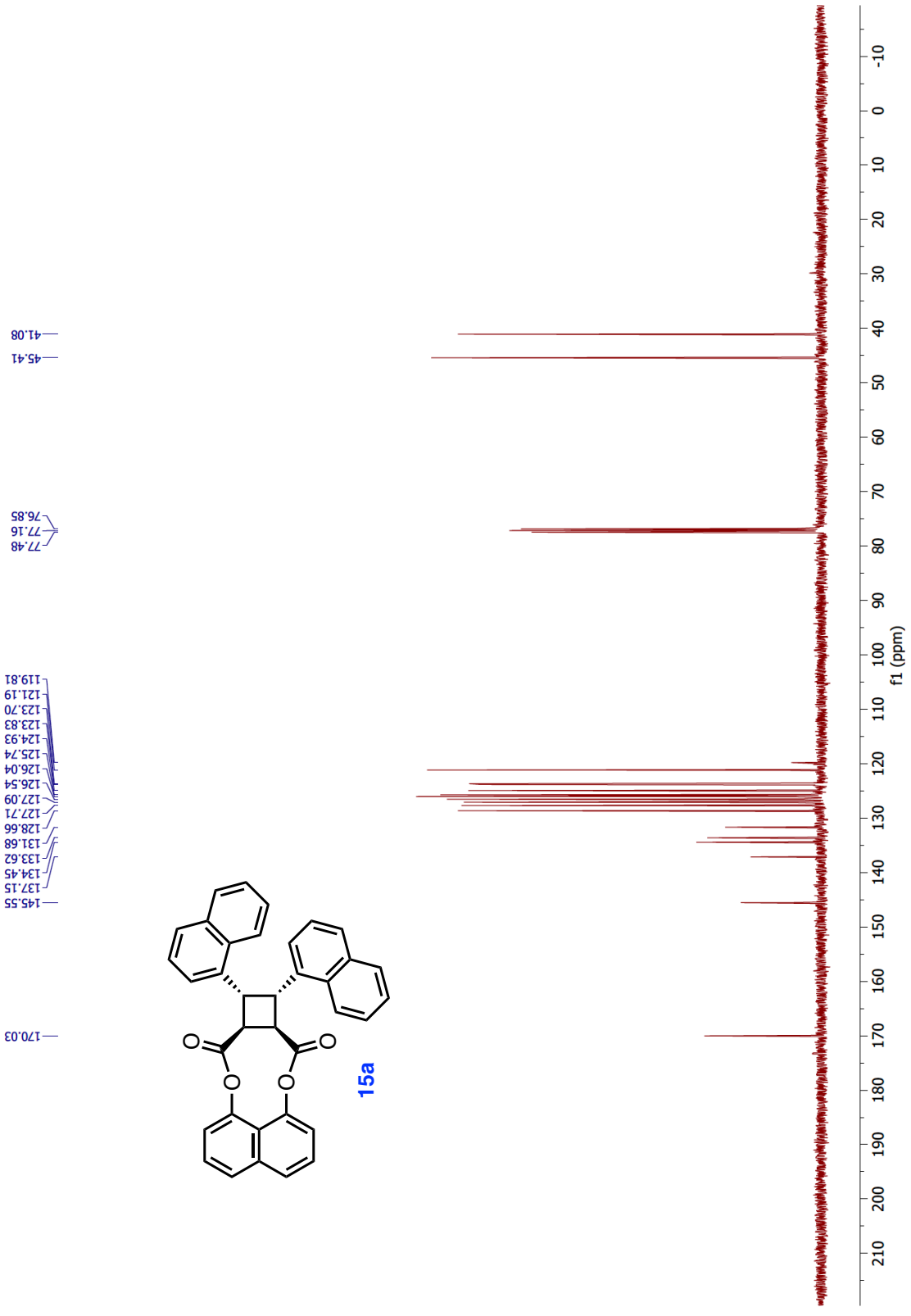


Figure S29. $^{13}C\{^{1}H\}$-NMR spectrum of **15a** in $CDCl_3$.

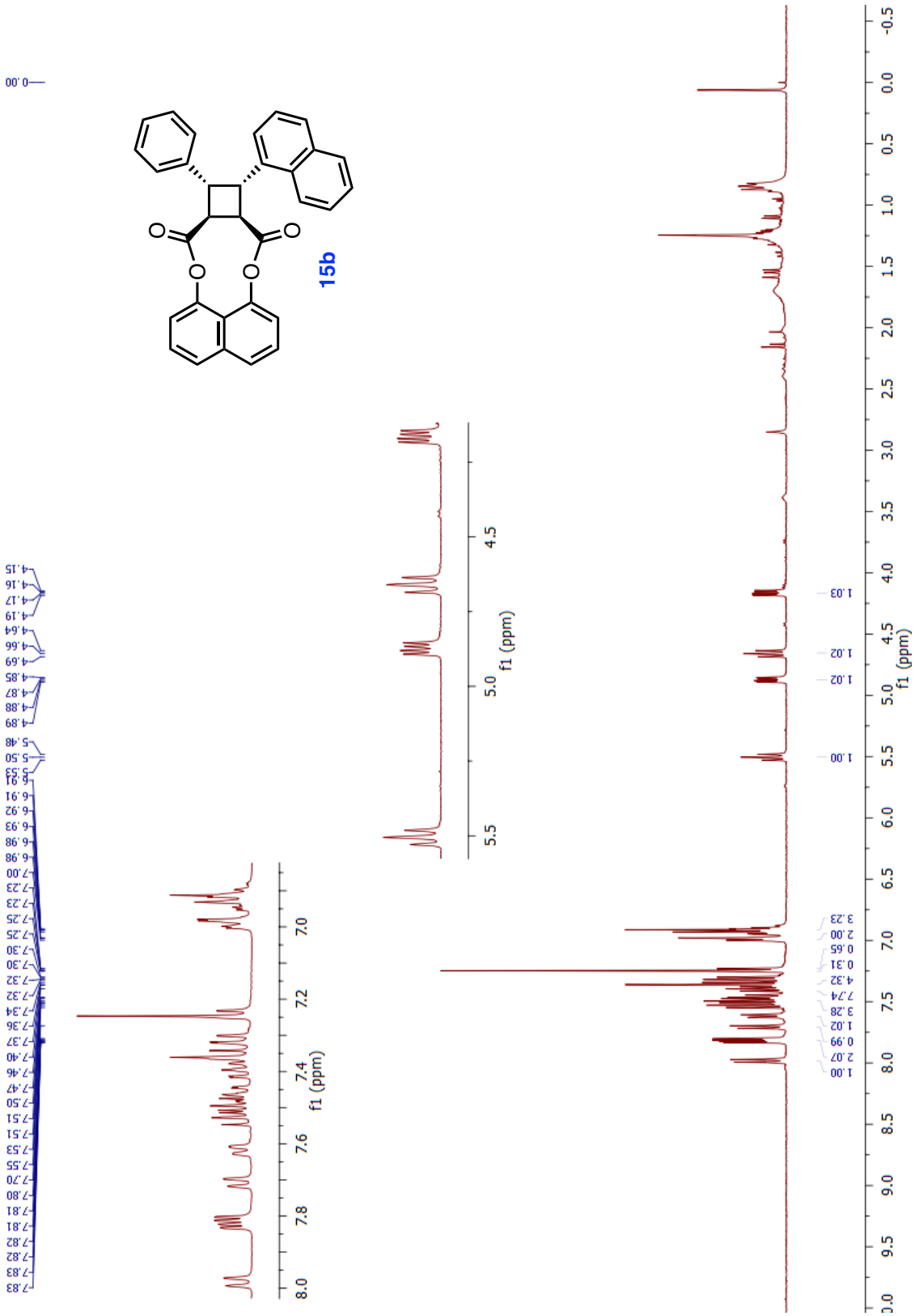


Figure S30. ^{1}H-NMR spectrum of **15b** in $CDCl_3$.

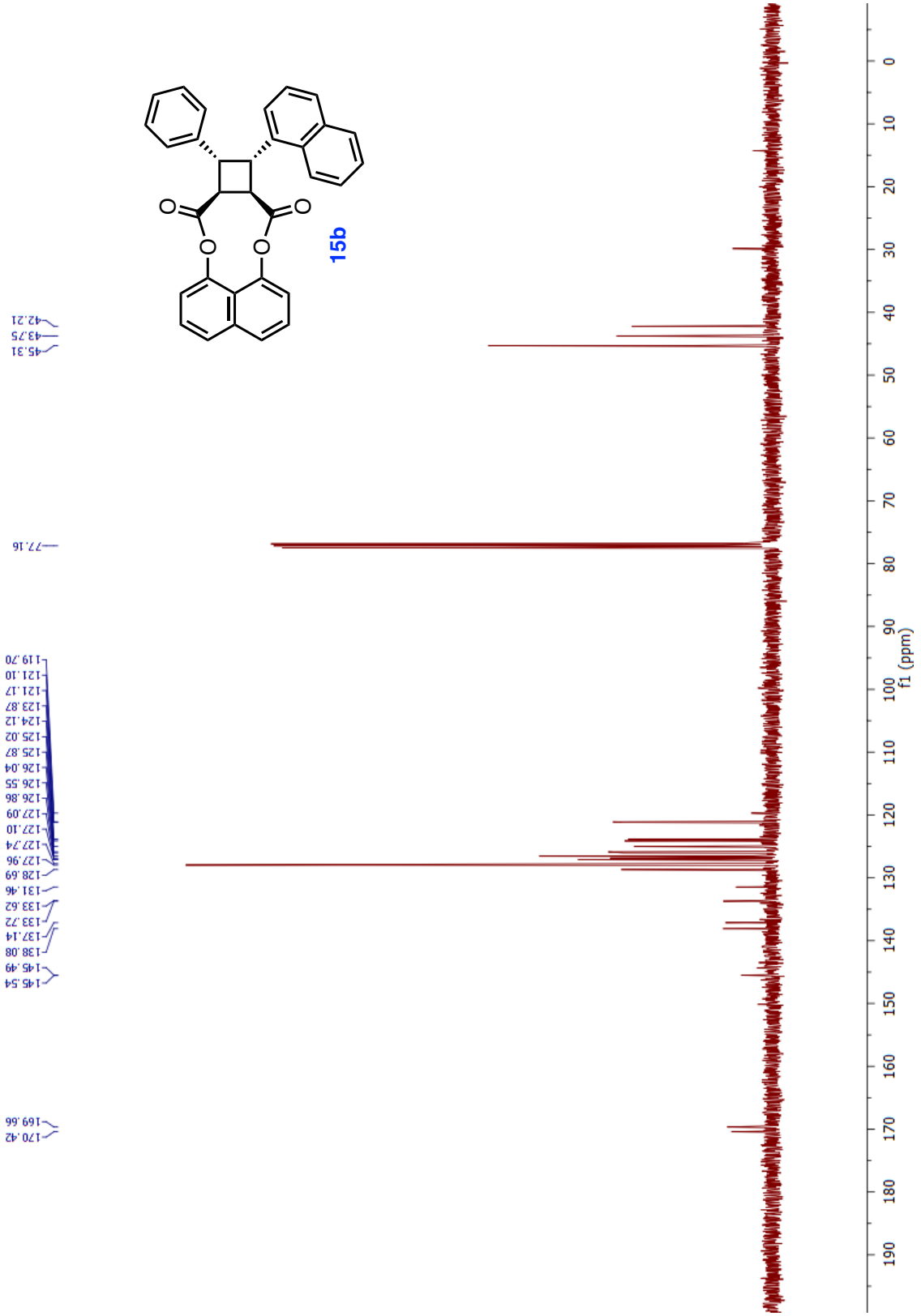


Figure S31. $^{13}C\{^{1}H\}$-NMR spectrum of **15b** in $CDCl_3$.

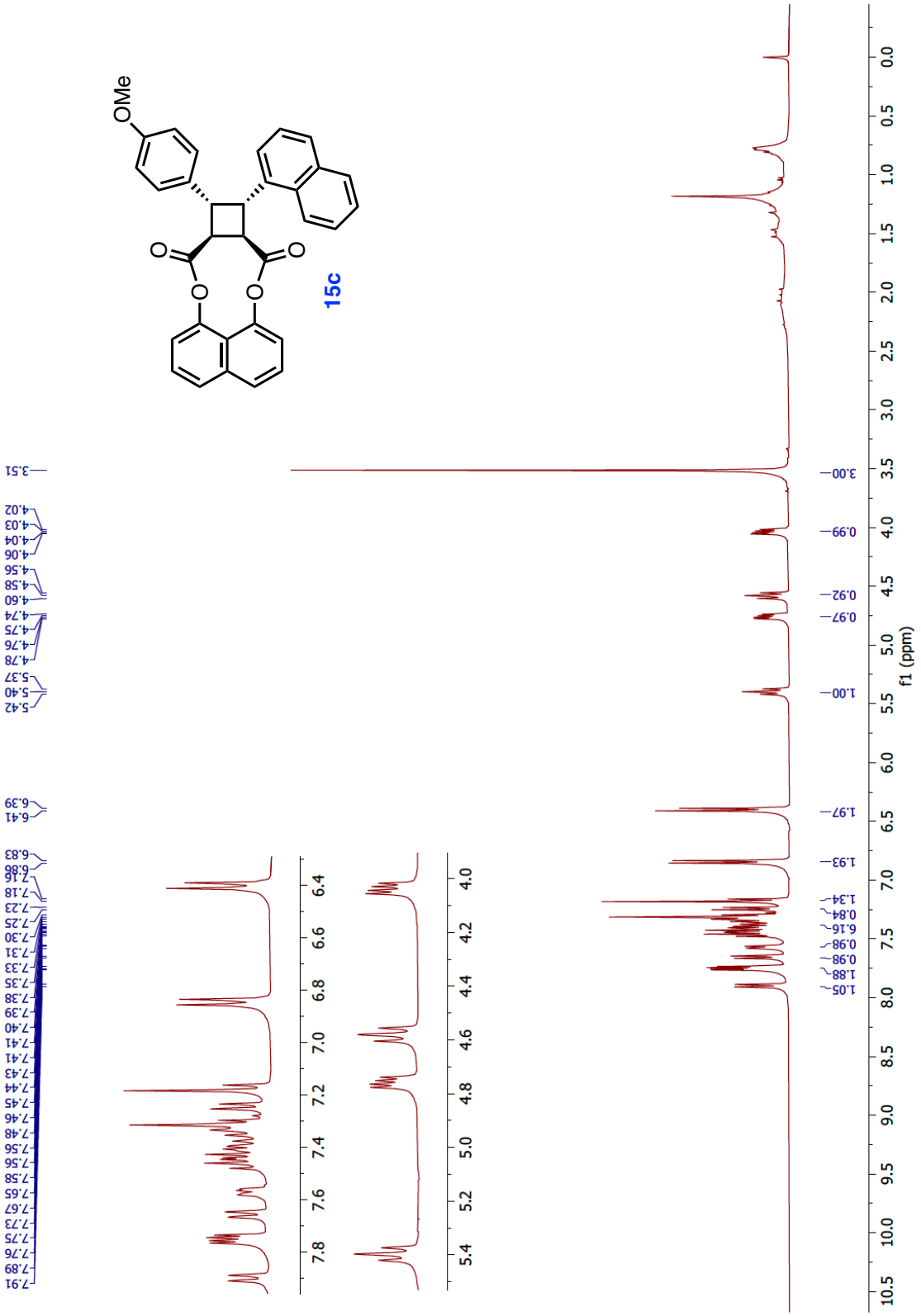


Figure S32. ^{1}H-NMR spectrum of **15c** in $CDCl_3$.

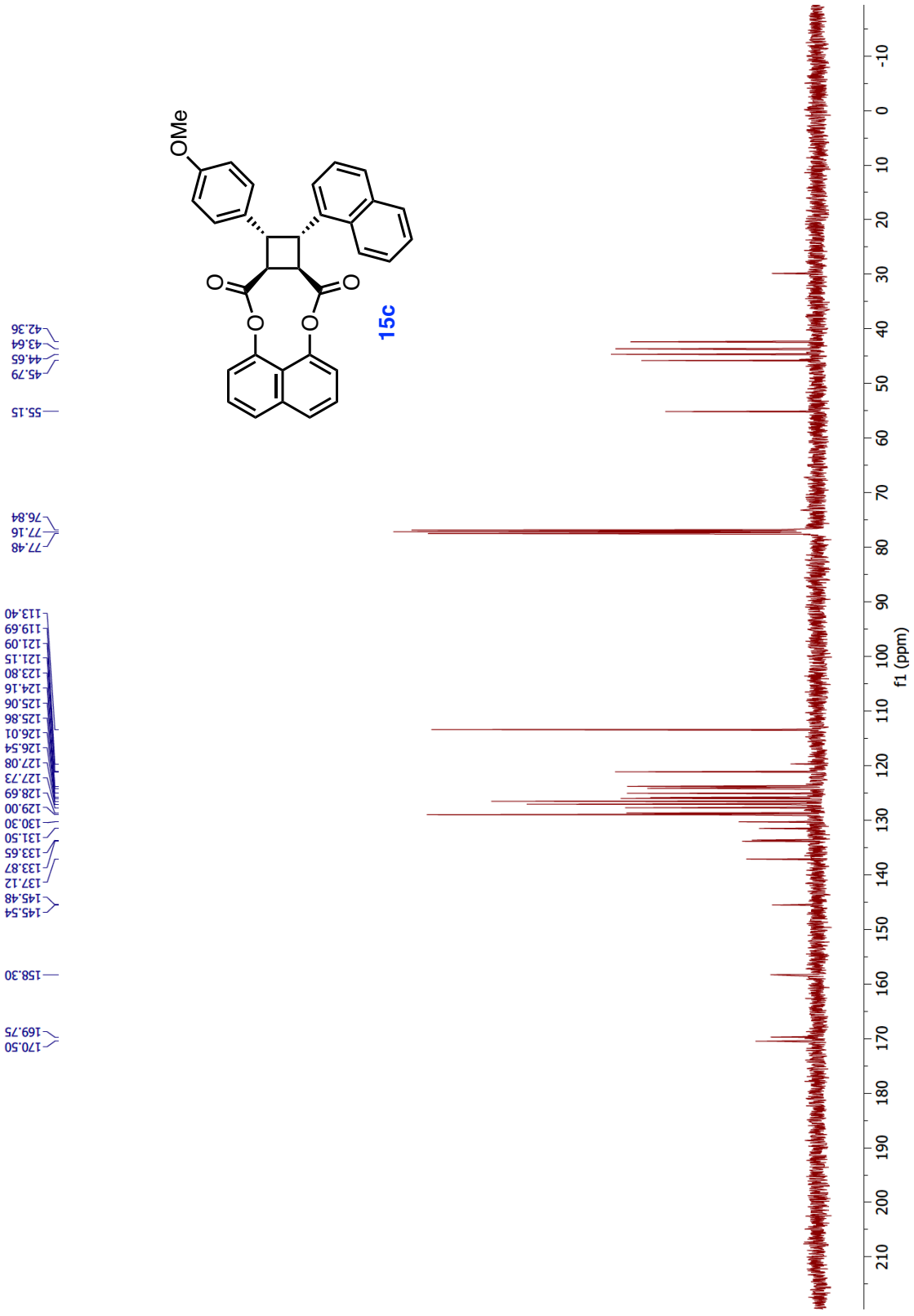


Figure S33. $^{13}C\{^{1}H\}$-NMR spectrum of **15c** in $CDCl_3$.

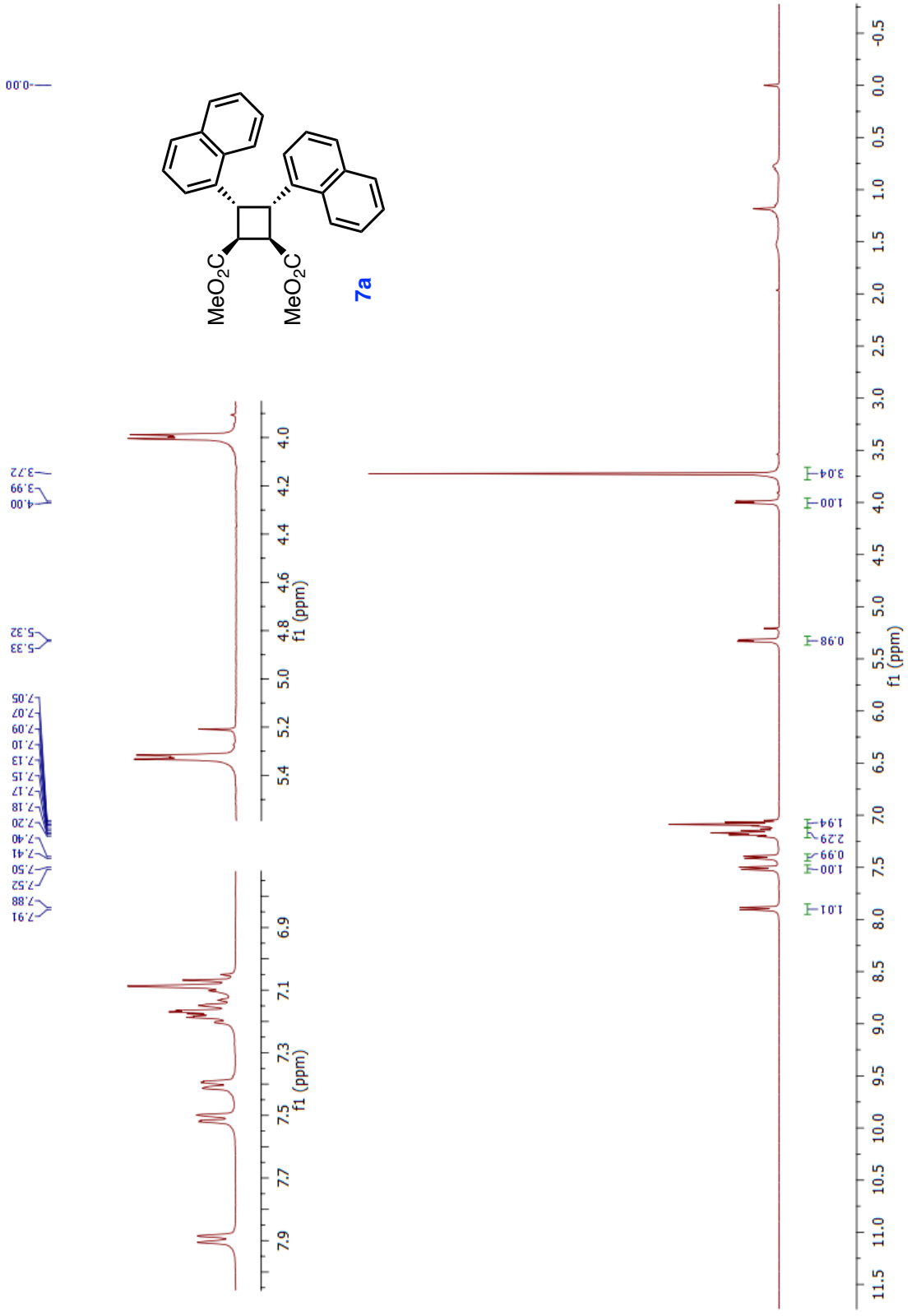


Figure S34. ^{1}H-NMR spectrum of **7a** in $CDCl_3$.

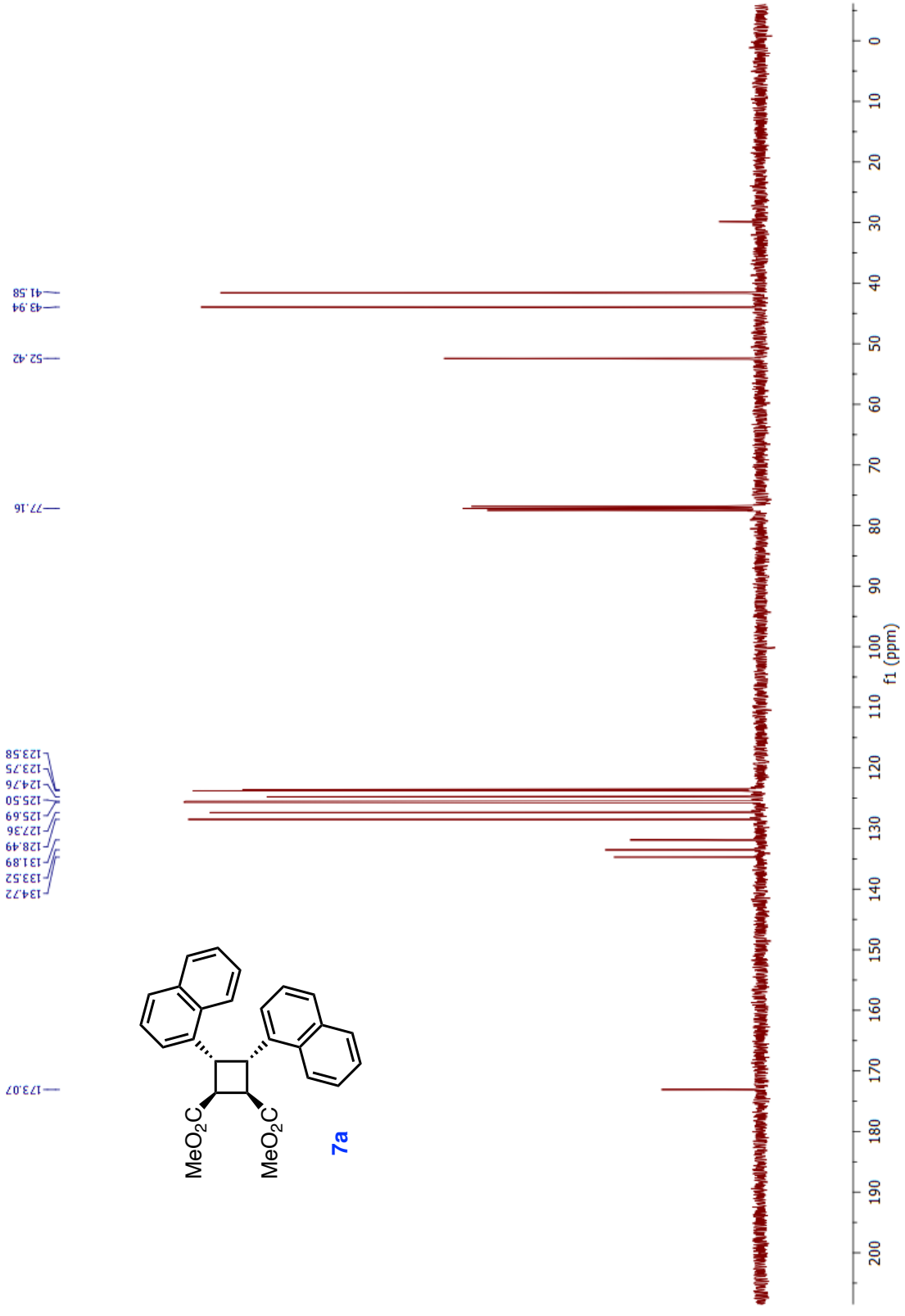


Figure S35. $^{13}C\{^{1}H\}$-NMR spectrum of **7a** in $CDCl_3$.

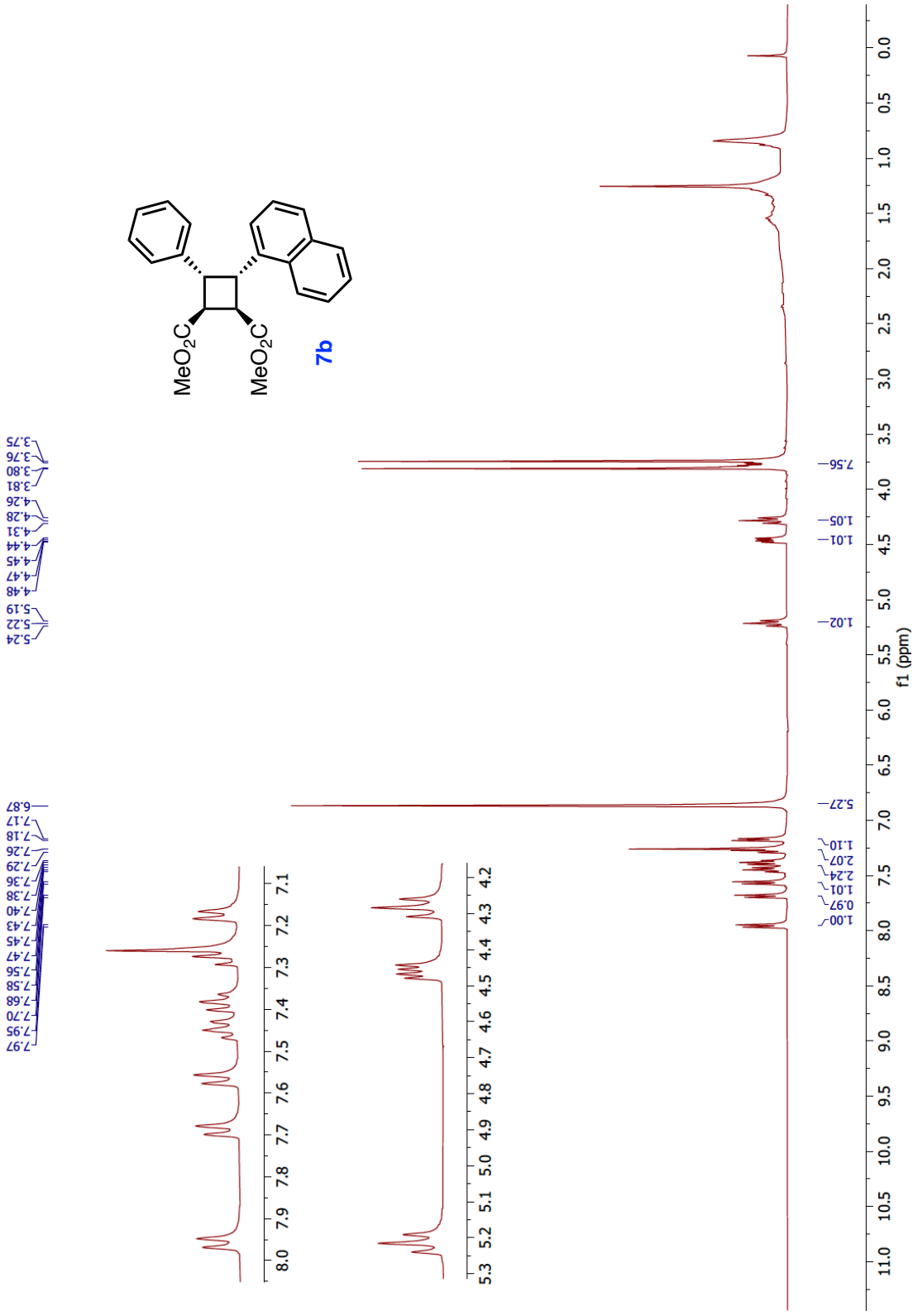


Figure S36. ^{1}H-NMR spectrum of **7b** in $CDCl_3$.

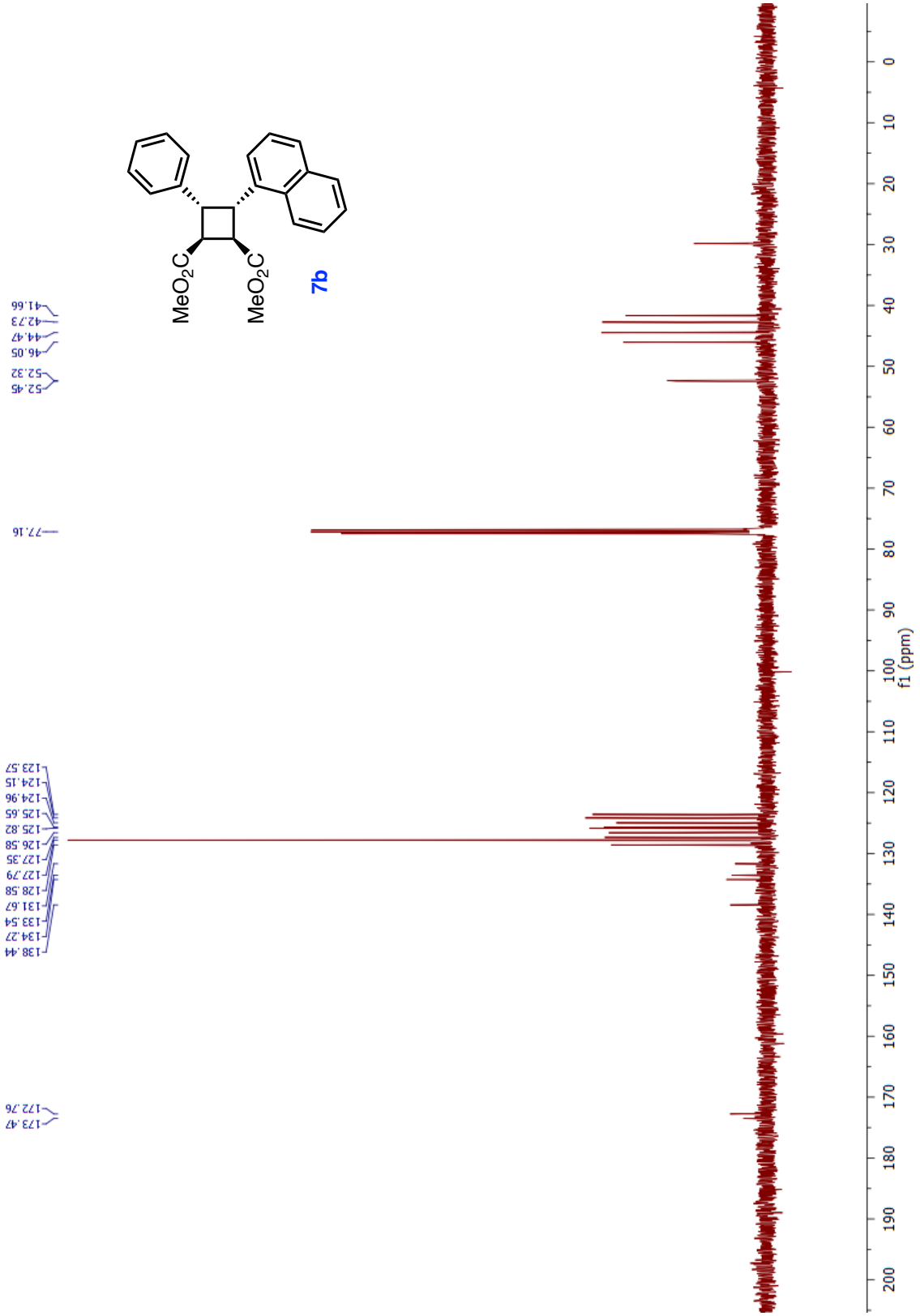


Figure S37. $^{13}C\{^{1}H\}$-NMR spectrum of **7b** in $CDCl_3$.

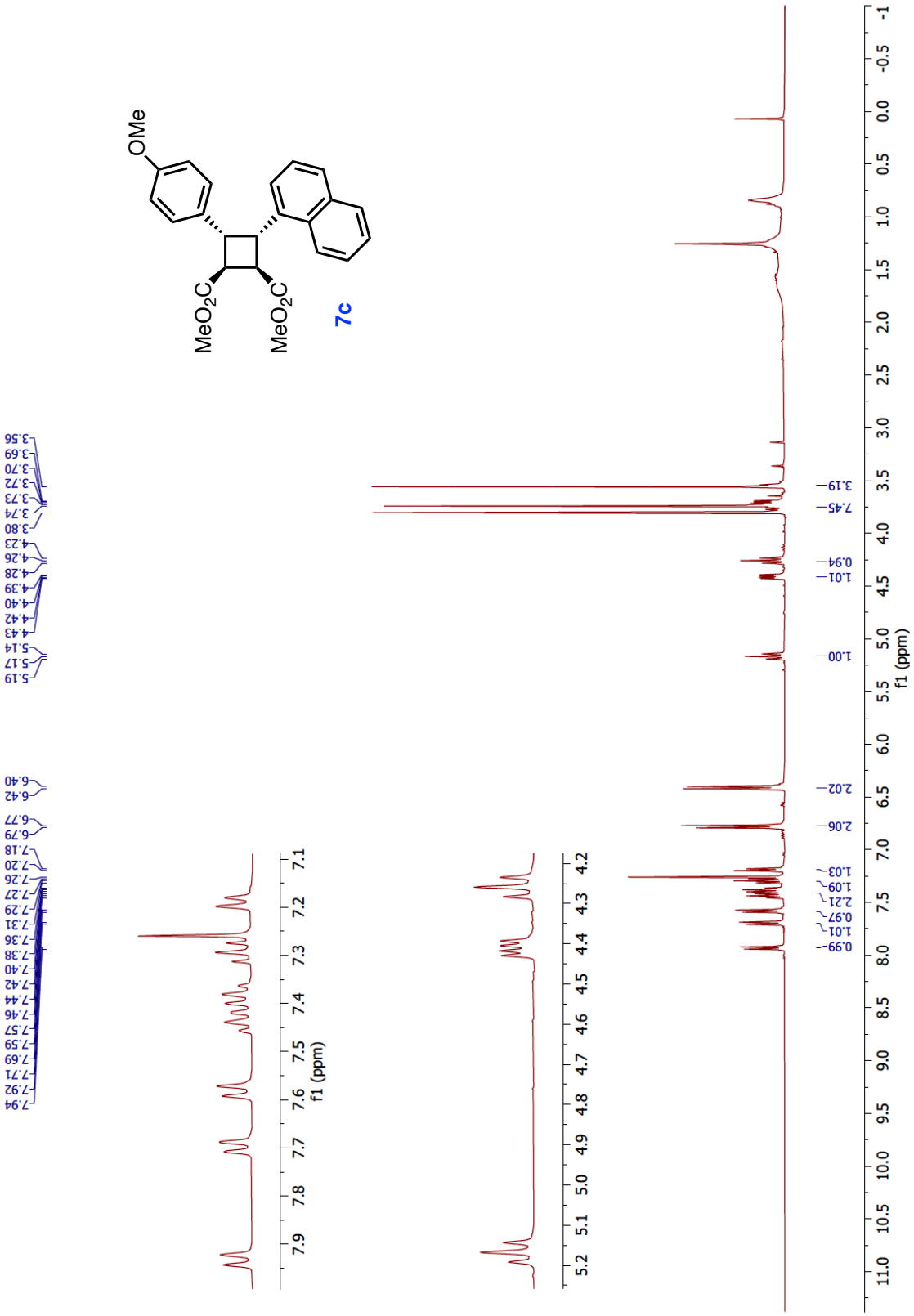


Figure S38. ^{1}H-NMR spectrum of **7c** in $CDCl_3$.

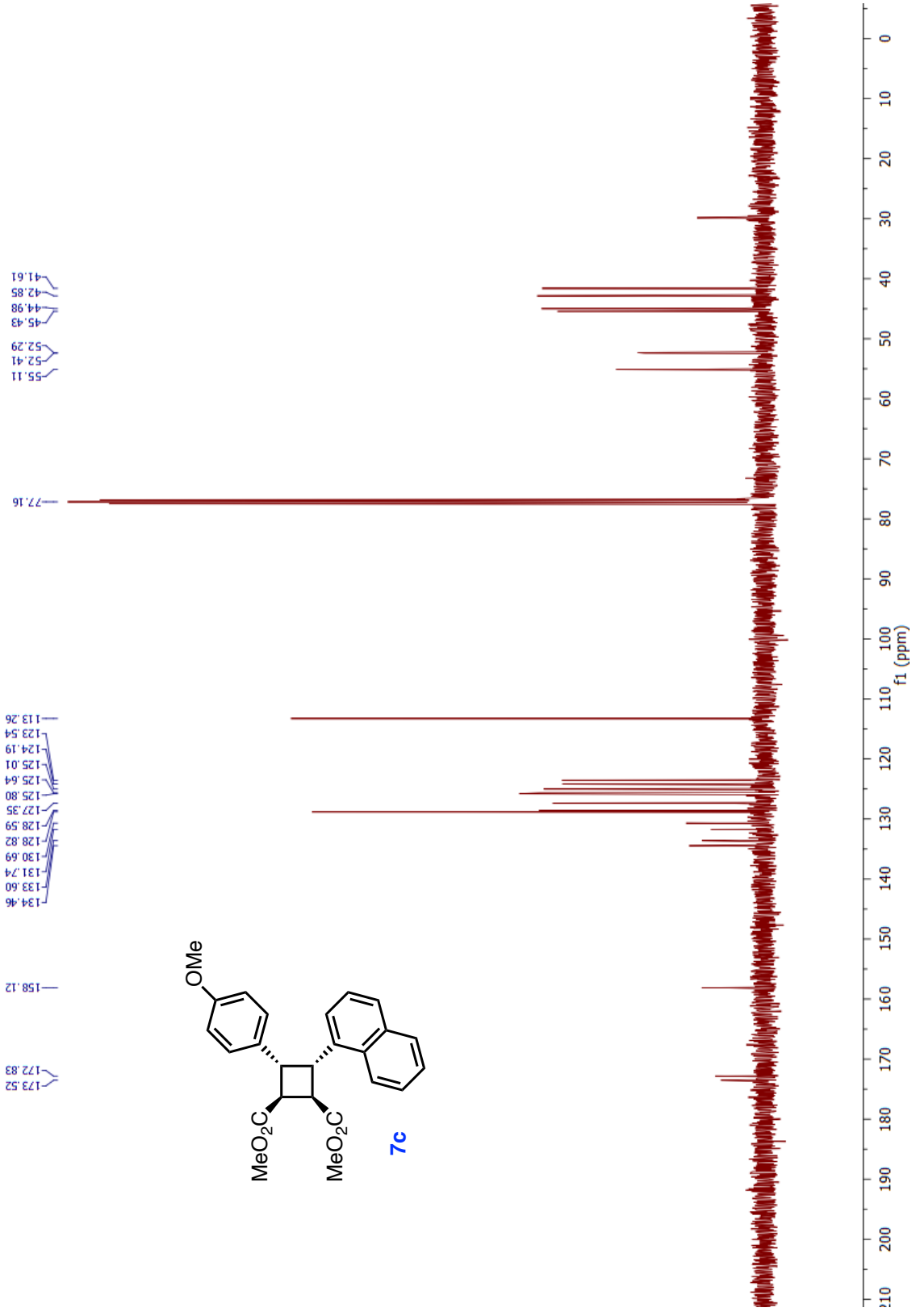


Figure S39. $^{13}C\{^{1}H\}$-NMR spectrum of **7c** in $CDCl_3$.

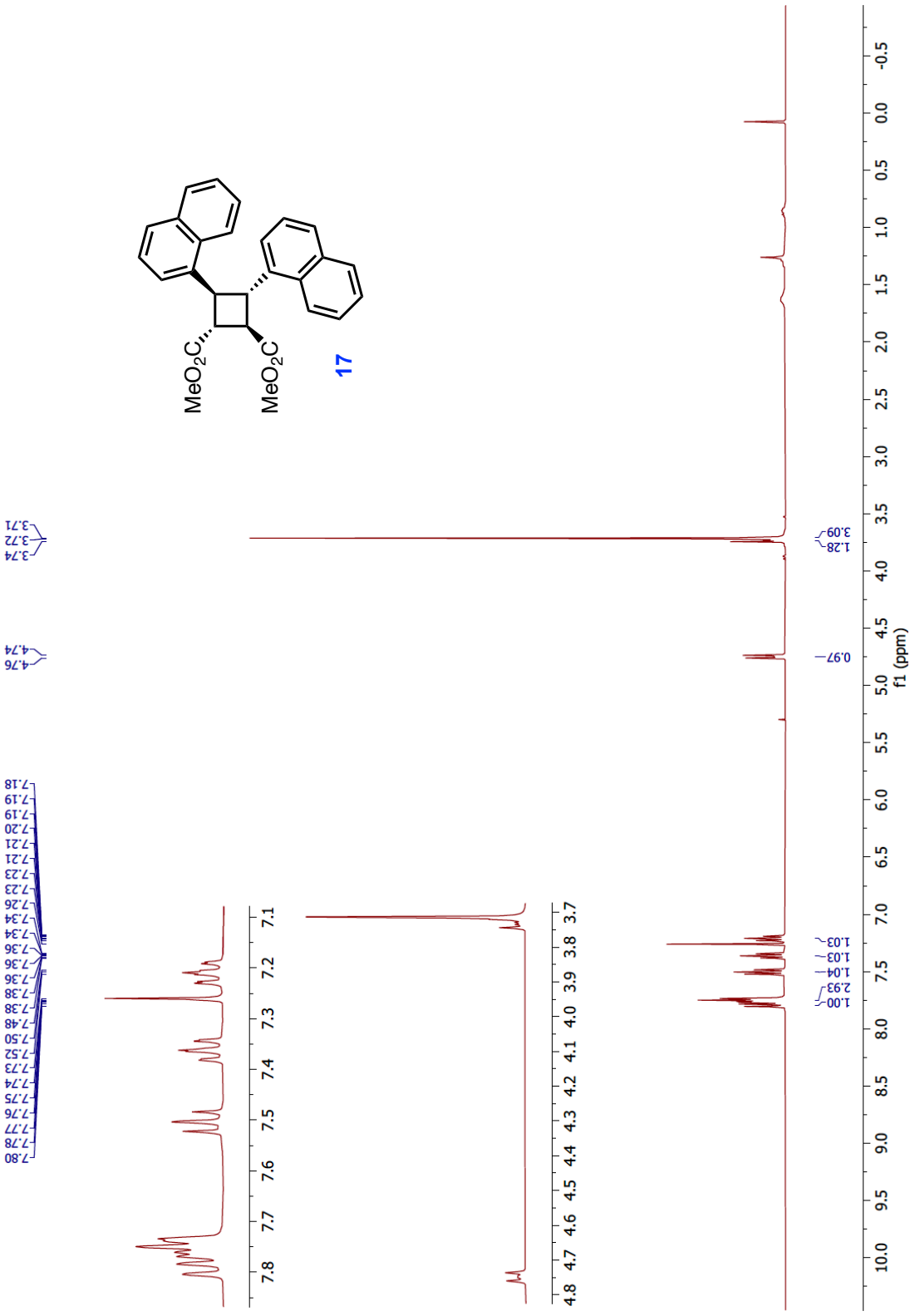


Figure S40. ^{1}H-NMR spectrum of **17** in $CDCl_3$.

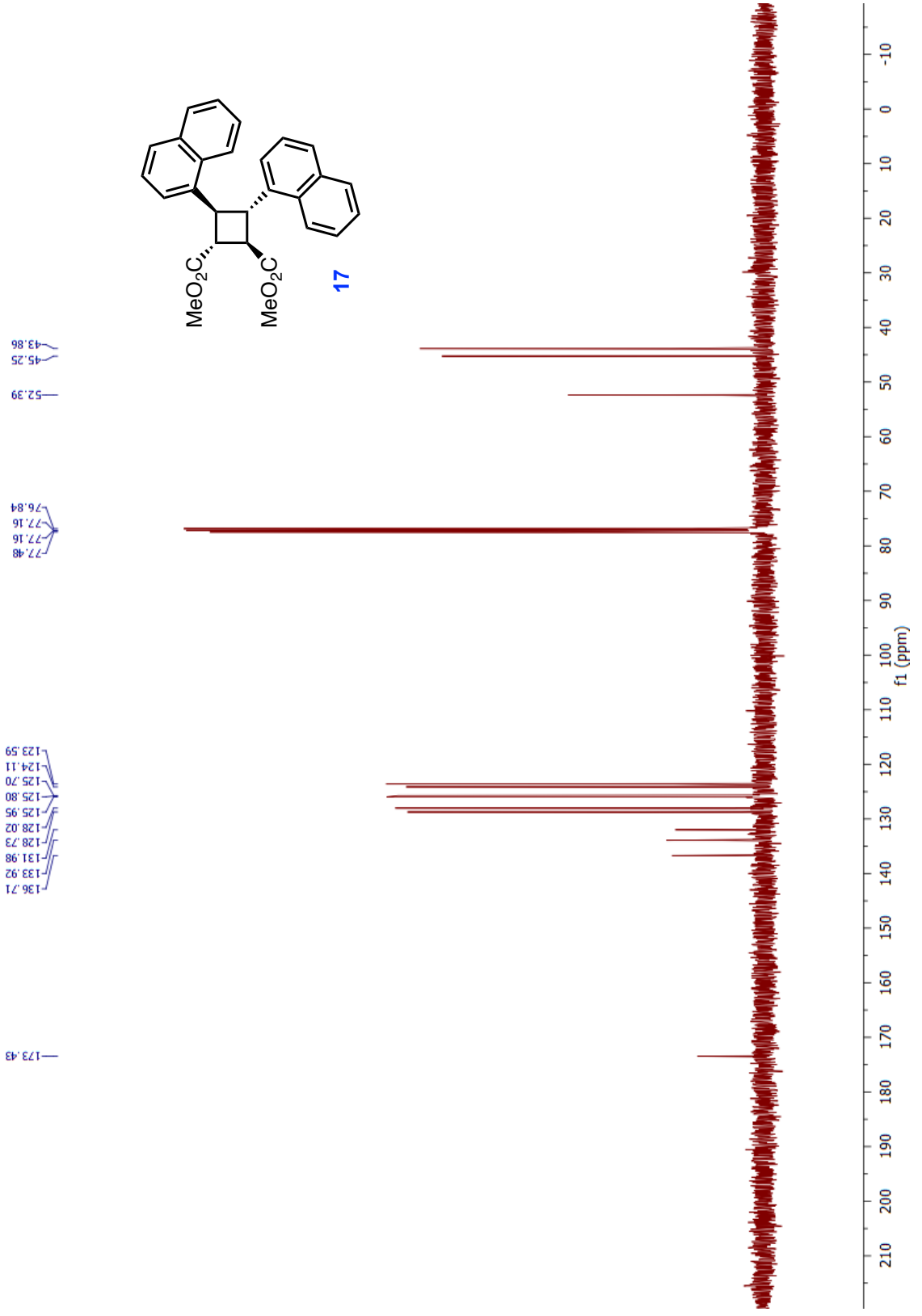


Figure S41. $^{13}C\{^{1}H\}$-NMR spectrum of **17** in $CDCl_3$.

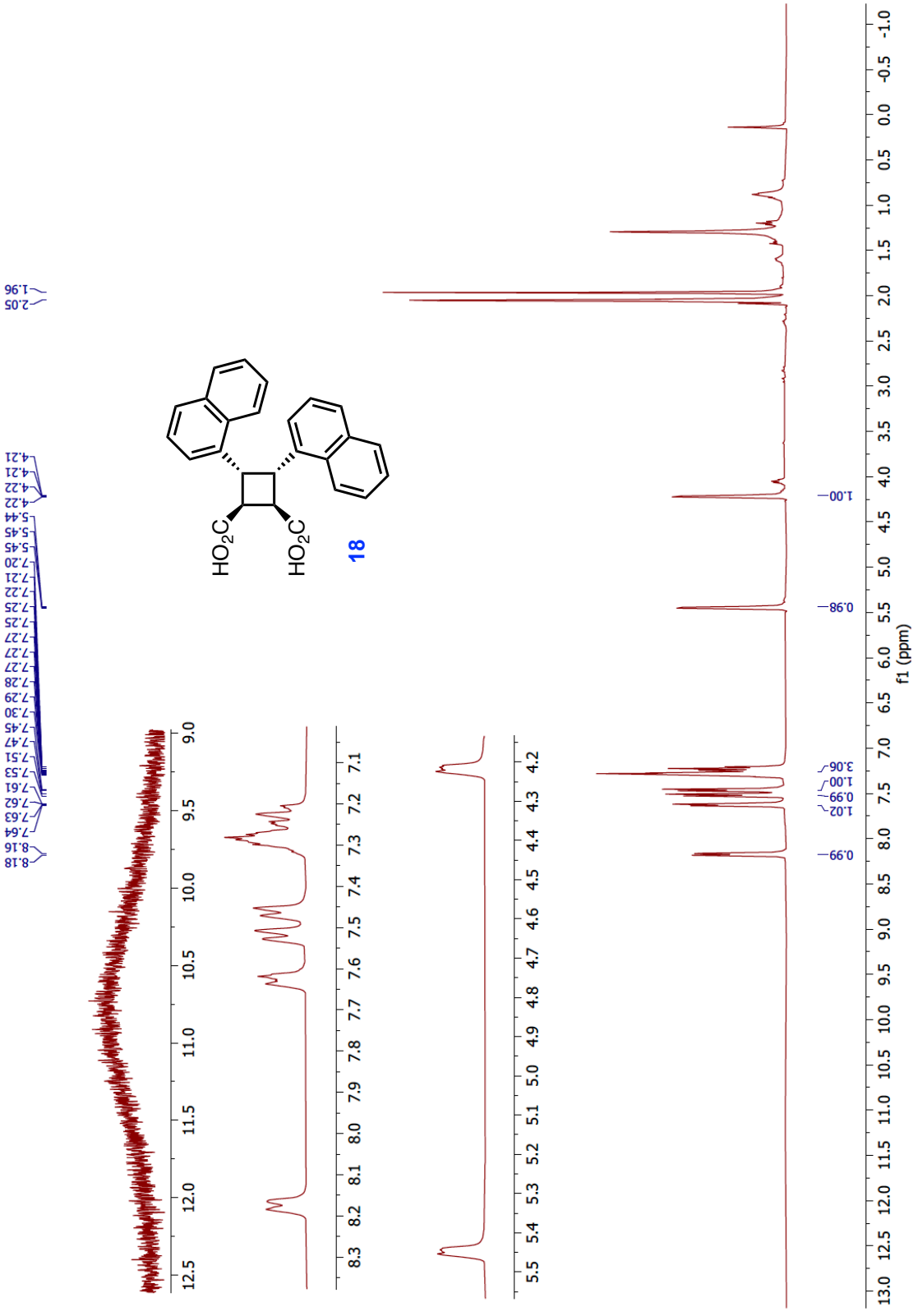


Figure S42. ^{1}H-NMR spectrum of **18** in acetone-d_6.

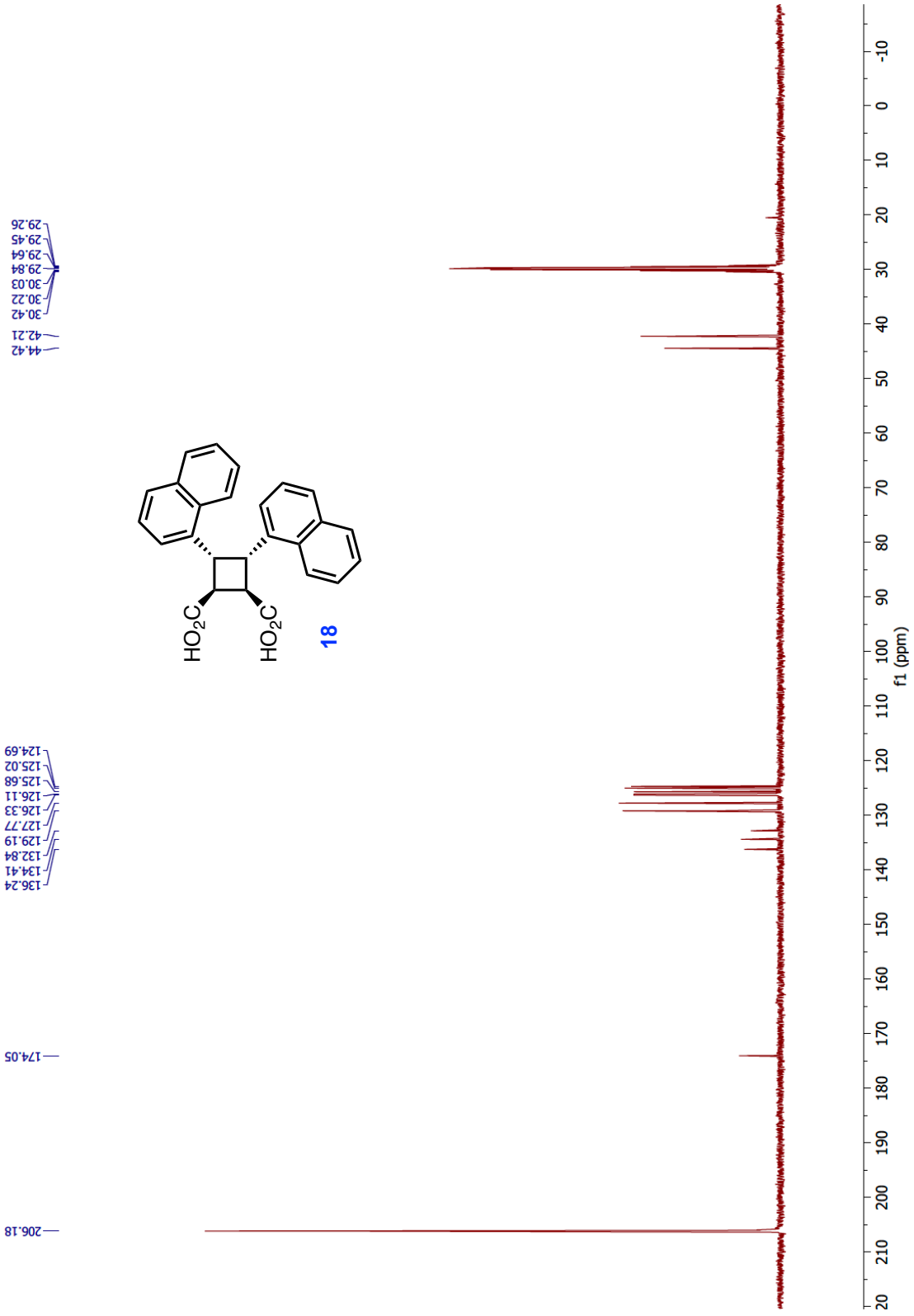


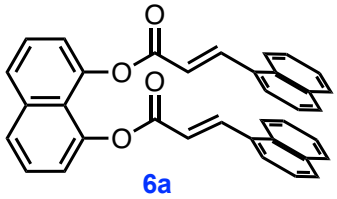
Figure S43. $^{13}C\{^{1}H\}$-NMR spectrum of **18** in acetone-d_6.

HRMS Data:

Qualitative Analysis Report

Data Filename	MT-3-45 01.d	**Sample Name**	MT-3-45
Sample Type	Sample	**Position**	vial 3
Instrument Name	Instrument 1	**User Name**	
Acq Method	without column.m	**Acquired Time**	9/10/2024 11:44:27 AM
IRM Calibration Status	Success	**DA Method**	111.m
Comment			

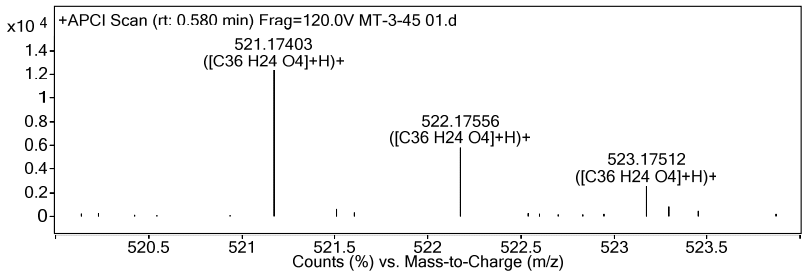
Method part to run:	Acquisition Only	**Sample Group Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)	**Stream Name**	LC 1



6a

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
120	0	APCI



Peak List

m/z	z	Abund
161.06172		94531.55
181.06457	1	189082.89
283.1328	1	53990.5
293.13824	1	51848.04
320.33056	1	76012.28
338.34103	1	1319262.88
339.34502	1	324334.91
340.3517	1	71682.16
407.20547	1	178140.38
419.20589	1	65176.21

Formula Calculator Element Limits

Element	Min	Max
C	35	36
H	23	24
O	4	4
N	0	0
Cl	0	0

Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C36 H24 O4	TRUE	520.1656	520.1675	3.54	C36 H25 O4	70.78

--- End Of Report ---

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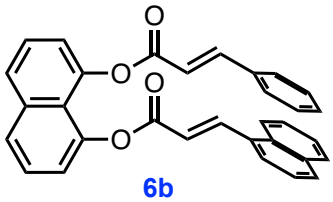
Qualitative Analysis Report

Data Filename	MT-3-109A 06.d	**Sample Name**	MT-3-109A
Sample Type	Sample	**Position**	vial 2
Instrument Name	Instrument 1	**User Name**	
Acq Method	without column.m	**Acquired Time**	9/2/2024 4:35:58 PM
IRM Calibration Status	Success	**DA Method**	111.m
Comment			

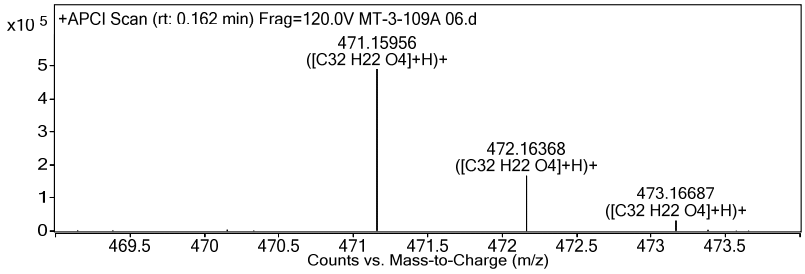
Method part to run:	Acquisition Only	**Sample Group Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)	**Stream Name**	LC 1



6b

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
120	0	APCI



Peak List

m/z	z	Abund	Formula	Ion
181.06547	1	2867777		
181.17854		228037.98		
182.06936	1	422371.94		
199.07683	1	367541.91		
213.09163	1	673020.25		
273.0925	1	447602.09		
323.10808	1	552968.63		
338.34319	1	605348.06		
361.22407	1	296854.81		
471.15956	1	495494.19	C32 H22 O4	(M+H)+

Formula Calculator Element Limits

Element	Min	Max
C	31	32
H	21	22
O	3	4
N	0	0
Cl	0	0

Formula Calculator Results

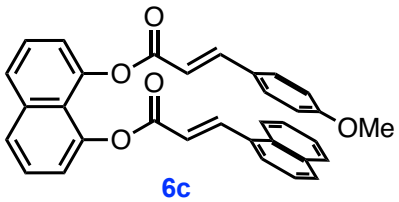
Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C32 H22 O4	TRUE	470.1525	470.1518	-1.48	C32 H23 O4	97.99

--- End Of Report ---

Qualitative Analysis Report

Data Filename	MT-3-117 12.d	**Sample Name**	MT-3-117
Sample Type	Sample	**Position**	vial 1
Instrument Name	Instrument 1	**User Name**	
Acq Method	without column.m	**Acquired Time**	9/10/2024 11:20:27 AM
IRM Calibration Status	Success	**DA Method**	111.m
Comment			

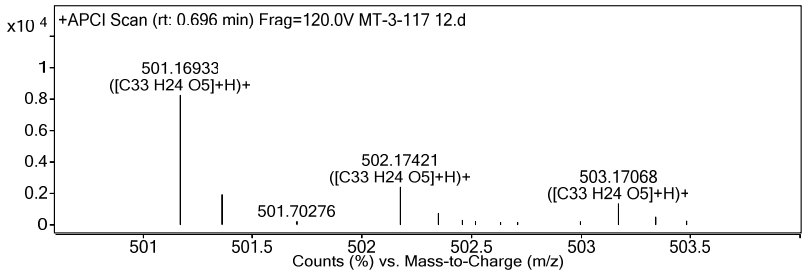
Method part to run:	Acquisition Only	**Sample Group Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)	**Stream Name**	LC 1



6c

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
120	0	APCI



Peak List

m/z	z	Abund
107.06001		81719.41
137.06218		39127.2
161.05901	1	292378.44
179.07369		38485.06
181.06374	1	43738.09
318.29947	1	48543.13
338.3407	1	497811.28
339.3437	1	116740.27
384.30748	1	56832.68
523.14792	1	67935.69

Formula Calculator Element Limits

Element	Min	Max
C	32	33
H	23	24
O	4	5
N	0	0
Cl	0	0

Formula Calculator Results

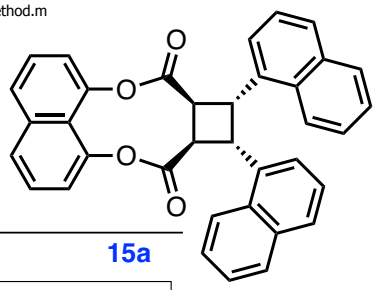
Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C33 H24 O5	TRUE	500.1618	500.1624	1.16	C33 H25 O5	72.55

--- End Of Report ---

Qualitative Analysis Report

Data Filename	MT-3-41 05.d	**Sample Name**	MT-3-41
Sample Type	Sample	**Position**	Vial 2
Instrument Name	Instrument 1	**User Name**	
Acq Method	without column.m	**Acquired Time**	6/5/2024 3:16:09 PM
IRM Calibration Status	Success	**DA Method**	QualDAMethod.m
Comment			

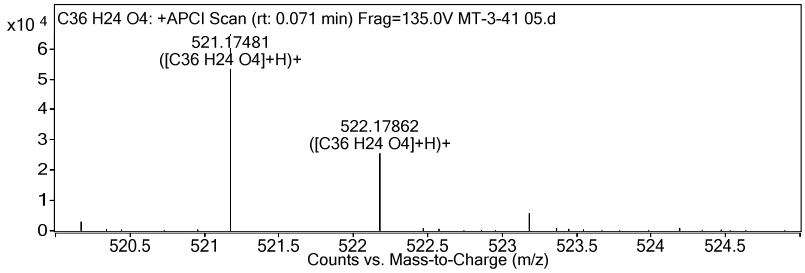
Method part to run:	Acquisition Only	**Sample Group Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)	**Stream Name**	LC 1



15a

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	APCI



Peak List

m/z	z	Abund	Formula	Ion
107.06165		60047.12		
150.12744		68444.3		
174.08886		38299.35		
265.10774	1	84591.02		
279.12228	1	50574.72		
295.11831	1	72216.79		
338.34281	1	66917.33		
481.19303	1	45306.92		
503.16449	1	36191.7		
521.17481	1	64909.12	C36 H24 O4	(M+H)+

Formula Calculator Element Limits

Element	Min	Max
C	35	36
H	23	25
O	2	4
N	0	0
S	0	0
Cl	0	0

Formula Calculator Results

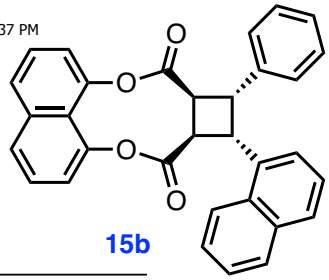
Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C36 H24 O4	TRUE	520.1678	520.1675	-0.58	C36 H25 O4	99.51

--- End Of Report ---

Qualitative Analysis Report

Data Filename	MT-3-112A 01.d	**Sample Name**	MT-3-112A
Sample Type	Sample	**Position**	vial1
Instrument Name	Instrument 1	**User Name**	
Acq Method	without column.m	**Acquired Time**	9/2/2024 3:27:37 PM
IRM Calibration Status	Success	**DA Method**	111.m
Comment			

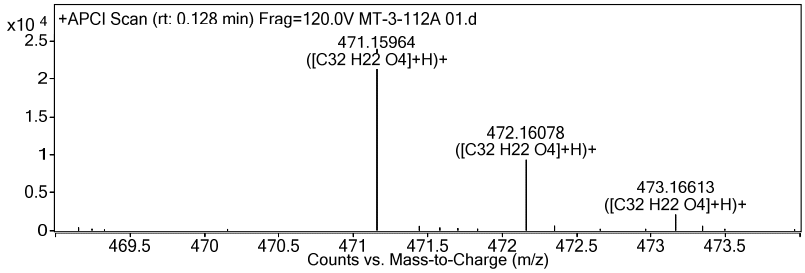
Method part to run:	Acquisition Only	**Sample Group Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)	**Stream Name**	LC 1



15b

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
120	0	APCI



Peak List

m/z	z	Abund	Formula	Ion
107.06041		30573.88		
122.07078		28488.01		
136.08331		21256.21		
137.08377		19208.81		
148.08572		18304.82		
149.0841		18329.48		
151.09719		17846.78		
163.09751		31223.11		
189.11226		19361.93		
471.15964	1	23930.24	C32 H22 O4	(M+H)+

Formula Calculator Element Limits

Element	Min	Max
C	31	32
H	21	22
O	3	4
N	0	0
Cl	0	0

Formula Calculator Results

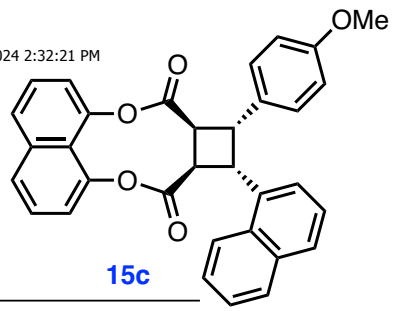
Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C32 H22 O4	TRUE	470.1516	470.1518	0.36	C32 H23 O4	94.42

--- End Of Report ---

Qualitative Analysis Report

Data Filename	MT-3-130 01.d	**Sample Name**	MT-3-130
Sample Type	Sample	**Position**	vial 1
Instrument Name	Instrument 1	**User Name**	
Acq Method	without column.m	**Acquired Time**	9/10/2024 2:32:21 PM
IRM Calibration Status	Success	**DA Method**	111.m
Comment			

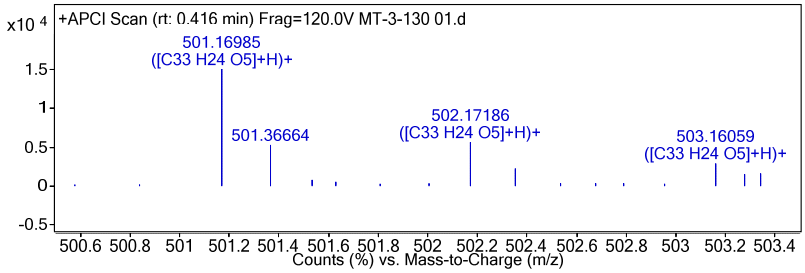
Method part to run:	Acquisition Only	**Sample Group**	
Info.		**Stream Name**	LC 1
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)		



15c

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
120	0	APCI



Peak List

m/z	z	Abund
241.04751	1	46860.24
273.16386	1	31605.78
274.27133	1	34983.88
318.29853	1	67329.45
338.33985	1	60062.8
384.305	1	102822.98
385.30255	1	39343.7
428.33119	1	52274.5
429.32301	1	29745.3
569.18881	1	39091.24

Formula Calculator Element Limits

Element	Min	Max
C	32	33
H	23	24
O	4	5
N	0	0
Cl	0	0

Formula Calculator Results

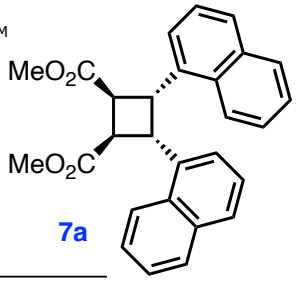
Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C33 H24 O5	TRUE	500.1604	500.1624	4	C33 H25 O5	64.52

--- End Of Report ---

Qualitative Analysis Report

Data Filename	MT-3-54 01.d	**Sample Name**	MT-3-54
Sample Type	Sample	**Position**	vial 2
Instrument Name	Instrument 1	**User Name**	
Acq Method	without column.m	**Acquired Time**	9/3/2024 11:41:53 AM
IRM Calibration Status	Success	**DA Method**	111.m
Comment			

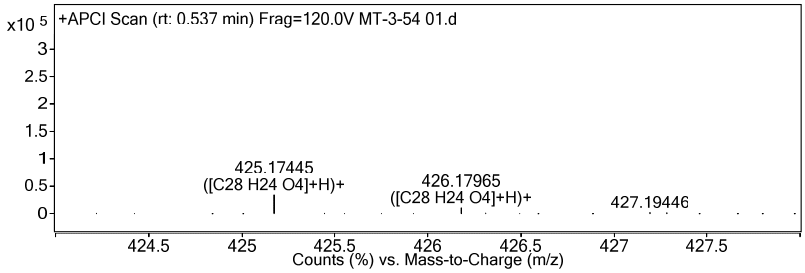
Method part to run:	Acquisition Only	**Sample Group**	
Info.		**Stream Name**	LC 1
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)		



7a

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
120	0	APCI



Peak List

m/z	z	Abund	Formula	Ion
181.06467	1	38875.48		
202.17914	1	97367.77		
325.22603	1	29079.51		
338.34159	1	30955.05		
361.12193	1	78389.82		
393.14853	1	282166.06		
394.15144	1	91287.41		
425.17445	1	34425.85	C28 H24 O4	(M+H)+
437.19572	1	27074.34		
485.35448	1	23215.6		

Formula Calculator Element Limits

Element	Min	Max
C	27	28
H	23	24
O	3	4
N	0	0
Cl	0	0

Formula Calculator Results

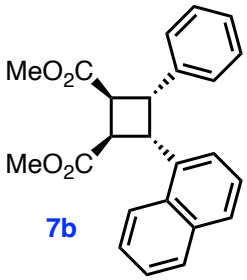
Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C28 H24 O4	TRUE	424.1676	424.1675	-0.33	C28 H25 O4	77.9

--- End Of Report ---

Qualitative Analysis Report

Data Filename	MT-3-126A 02.d	**Sample Name**	MT-3-126A
Sample Type	Sample	**Position**	vial 2
Instrument Name	Instrument 1	**User Name**	
Acq Method	without column.m	**Acquired Time**	9/10/2024 2:57:39 PM
IRM Calibration Status	Success	**DA Method**	111.m
Comment			

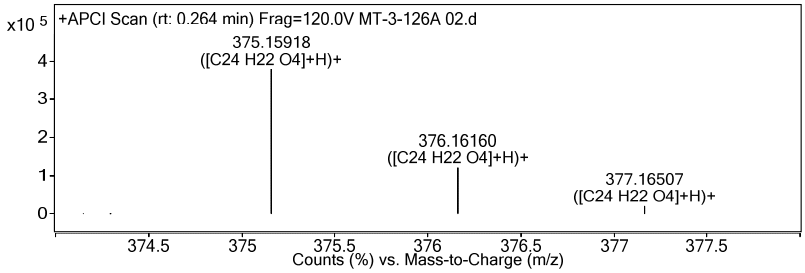
Method part to run:	Acquisition Only	**Sample Group Info.**	
Stream Name	LC 1		
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)		



7b

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
120	0	APCI



Peak List

m/z	z	Abund	Formula	Ion
311.10642	1	2074763.25		
312.10977	1	508240.84		
315.13825	1	157040.53		
338.34132	1	177766.7		
343.13325	1	5665070.5		
344.13547	1	1616610.88		
345.13914	1	245792.88		
375.15918	1	5047771	C24 H22 O4	(M+H)+
376.1616	1	1498595.25	C24 H22 O4	(M+H)+
377.16507	1	246439.81	C24 H22 O4	(M+H)+

Formula Calculator Element Limits

Element	Min	Max
C	23	24
H	21	22
O	3	4
N	0	0
Cl	0	0

Formula Calculator Results

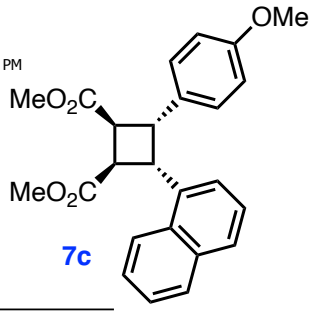
Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C24 H22 O4	TRUE	374.1517	374.1518	0.35	C24 H23 O4	96.91

--- End Of Report ---

Qualitative Analysis Report

Data Filename	MT-3-134A 02.d	**Sample Name**	MT-3-134A
Sample Type	Sample	**Position**	vial 4
Instrument Name	Instrument 1	**User Name**	
Acq Method	without column.m	**Acquired Time**	9/10/2024 12:15:53 PM
IRM Calibration Status	Success	**DA Method**	111.m
Comment			

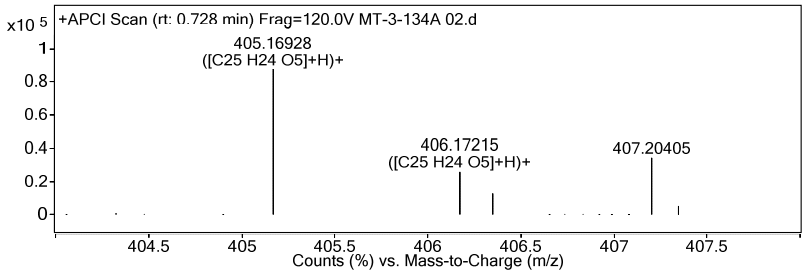
Method part to run:	Acquisition Only	**Sample Group**	
Info.		**Stream Name**	LC 1
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)		



7c

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
120	0	APCI



Peak List

m/z	z	Abund	Formula	Ion
274.27422	1	148086.89		
318.30091	1	375509		
338.34139	1	254254.52		
340.28419	1	95083.91		
362.3257	1	175716.27		
373.14379	1	258797.64		
384.30742	1	649270.31		
385.3106	1	154223.02		
405.16928	1	219015.27	C25 H24 O5	(M+H)+
428.33394	1	260083.98		

Formula Calculator Element Limits

Element	Min	Max
C	24	25
H	23	24
O	4	5
N	0	0
Cl	0	0

Formula Calculator Results

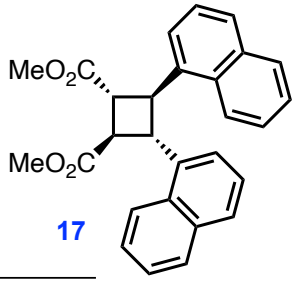
Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C25 H24 O5	TRUE	404.1619	404.1624	1.2	C25 H25 O5	81.3

--- End Of Report ---

Qualitative Analysis Report

Data Filename	MT-3-82A 01.d	**Sample Name**	MT-3-82A
Sample Type	Sample	**Position**	vial 1
Instrument Name	Instrument 1	**User Name**	
Acq Method	without column.m	**Acquired Time**	9/3/2024 11:15:54 AM
IRM Calibration Status	Success	**DA Method**	111.m
Comment			

Method part to run:	Acquisition Only	**Sample Group**	
Info.		**Stream Name**	LC 1
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)		



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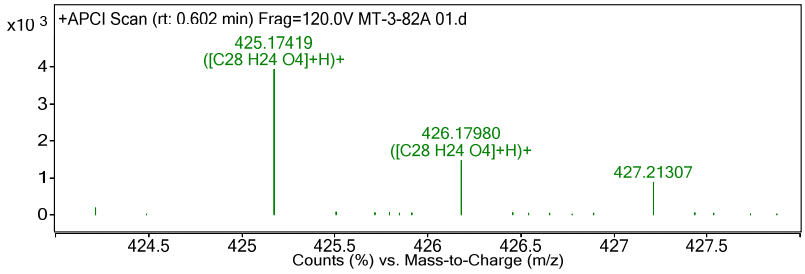
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
120	0	APCI



Peak List

m/z	z	Abund	Formula	Ion
325.22358	1	31933.92		
338.33681	1	15046.79		
361.12684	1	12338.59		
385.28656	1	11333.17		
393.14524	1	36061.45		
394.14825	1	10451.59		
425.17419	1	15281.99	C28 H24 O4	(M+H)+
429.31201	1	11467.13		
437.19435	1	10210.13		
481.18794	1	13694.09		

Formula Calculator Element Limits

Element	Min	Max
C	27	28
H	23	24
O	3	4
N	0	0
Cl	0	0

Formula Calculator Results

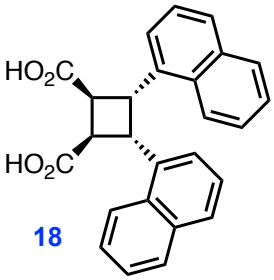
Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C28 H24 O4	TRUE	424.1675	424.1675	-0.07	C28 H25 O4	73.27

--- End Of Report ---

Qualitative Analysis Report

Data Filename	MT-3-77A 06.d	**Sample Name**	MT-3-77A
Sample Type	Sample	**Position**	vial 1
Instrument Name	Instrument 1	**User Name**	
Acq Method	without column.m	**Acquired Time**	9/9/2024 3:23:19 PM
IRM Calibration Status	Success	**DA Method**	111.m
Comment			

Method part to run:	Acquisition Only	**Sample Group Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)	**Stream Name**	LC 1



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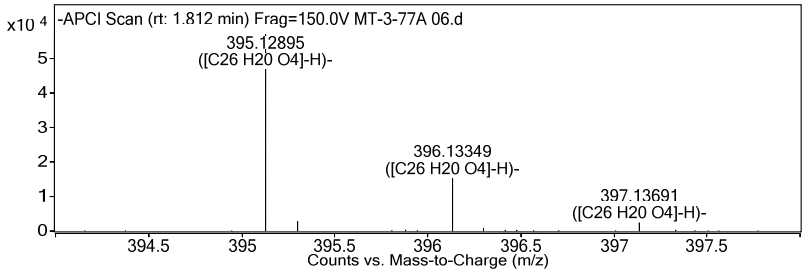
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	APCI



Peak List

m/z	z	Abund	Formula	Ion
106.04226		9234.5		
121.03075		10058.13		
126.90437		60413.04		
138.02033		5264.3		
143.10756	1	41565.14		
144.10975	1	5088.49		
248.9727		4710.74		
395.12895	1	56965.76	C26 H20 O4	(M-H)-
396.13349	1	15193.51	C26 H20 O4	(M-H)-
813.24522	1	7844.65		

Formula Calculator Element Limits

Element	Min	Max
C	24	26
H	19	20
O	3	4
N	0	0
Cl	0	0

Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Ion Species	Score
C26 H20 O4	TRUE	396.1365	396.1362	-0.89	C26 H19 O4	97.51

--- End Of Report ---