Supporting information for:

Synthesis of 2,6-Diaminotriptycene Conjugates with Chiral Auxiliaries: Towards the Scalable Resolution of Crucial Triptycene Intermediates

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1. Chromatographic analyses.

HESI determinations were performed with MS spectrometer Thermo Scientific (Milan, Italy) LTQ XL HESI-MS/MS system using direct injection of purified fractions. HESI Probe: Gas = N_2, T = 70°C, Voltage=3.6 kV; Capillary T = 275°C, Voltage = 48V, Tube Lens=70V. Tune Settings: Multipole 00 Offset = 2.5V, Lens 0 = -4.28V, Multipole 0 Offset = -5.12V, Lens 1 = - 8.91, Gate Lens = - 66.1V, Multipole 1 Offset = - 6.5V, Multipole RF Amplitude (p-p)= 400V, Front Lens = - 6.1V. Settings for MS-MS and MS^3: detection by CID (Collision Induced Dissociation); Isolation Width: ±2 amu; Activation Q: 0.250; Activation Time 30.0 msec. Isolation width for quantitation ±2.5 amu.

UHPLC analysis were carried out using: Instrument: The chromatographic analysis was performed with a UHPLC apparatuts JASCO (Lecco, Italy) X-LC system coupled with a MS spectrometer Thermo Scientific (Milan, Italy) LTQ XL HESI-MS/MS system. The column used for chromatographic separation was a RESTEK Raptor ®, RP-C18 column id = 2.1 mm, length = 50 mm and particle size = 1.8 μm (equipped with a similar pre-column). After an equilibration period of 5 min, 2-5 μL of each sample were injected in the UPLC system. Isocratic elution was performed with acetonitrile/water–0.2%HCOOH (10:90) as a mobile phase, the flow rate was 0.3 mL min^{-1} for 1 min, gradient was increased to 100% acetonitrile after 10 min. The column temperature was maintained at 40 °C with "on-line" oven equipment, and the total run time was 15 min (including a 4 min of column washing performed with pure ACN at same flow). To obtain best performance for separation the samples were tested with more powerful Raptor ®, RP-C18 column id = 2.1 mm, length = 100 mm and particle size = 1.8 μm. The HPLC analysis with chiral analytical column were carried out using Shimadzu HPLC for standard mobile phases and JASCO HPLC/SFC instruments equipped with chiral column. The results are summarized in the table below.

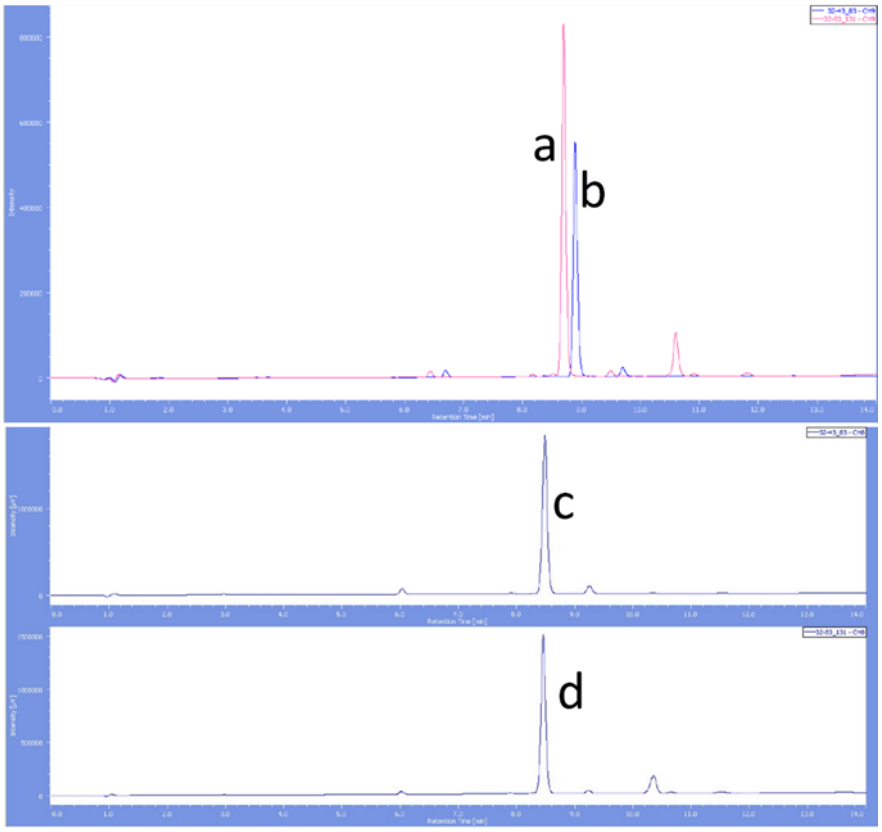

Figure S1. UHPLC analysis of the ffirst (**a** or **c**) and last (**b** or **d**) eluting fractions of **1d** from flash column chromatography by injecting 1 microliter of a 0.25 mg/mL solution of analyte (**a** and **b**) or 3 microliters of a 0.75 mg/mL solution of analyte (**c** and **d**).

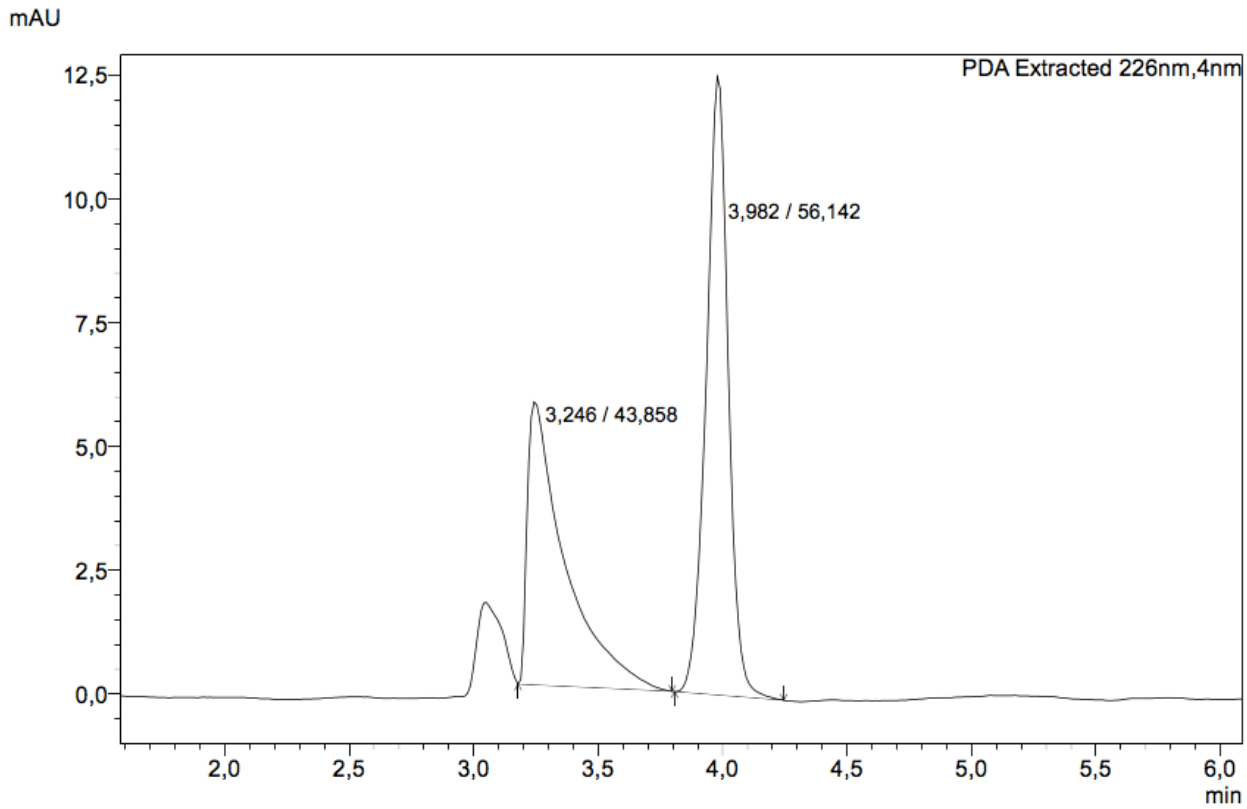

Figure S2. HPLC trace of compound **1b** obtained with Chiralcel® OD-3 phase. HPLC conditions: Flow 1 mL/min, eluent: 98:2 *n*Heptane-*iso*PrOH, extraction at maximum absorbance (226 nm) of compound **1b**. Solution 5 mg/mL, injection = 15 µL.

Table S1. Bad = bad separation, undefined peaks; Poor = poor separation, not resolved peaks; Acceptable = low separation with identified peaks; Good = nice separation. Separated with Raptor ® RP18 UHPLC column.

Compound/Conditions	**Chirapak® AS-H**	**Chiralcel® OD-3**	**Chirapak® IA-3**	**Chirapak® IB-3**	**Chirapak® IC-3**	**UHPLC Restek Raptor**
1a	Bad	Bad	Bad	Bad	Bad	Single peak
1b	Bad	Acceptable	Poor	bad	bad	Poor
1c	Bad	Poor	Poor	Bad	Bad	Single peak
1d	Bad	Bad	Bad	Bad	Bad	Good
1e	Bad	Poor	Poor	Bad	Bad	Single peak

2. Computational details

Product conformers search. The product structures utilized in the study were prepared using GaussView6 software and underwent a manual conformational sampling towards all the possible rotamers of both the amidic bonds and the ramification within the molecular structure of the chiral auxiliary. Both C_2 symmetrical and unsymmetrical systems were investigated. The so obtained conformers where then subjected to the low level of theory optimization and the most stable ones were than involved in the single point calculation to account for the role of solvent. The weight of conformations that do not show C_2 symmetry (**1-d-a** and **1-d'-c**) was counted twice for statistical reasons.

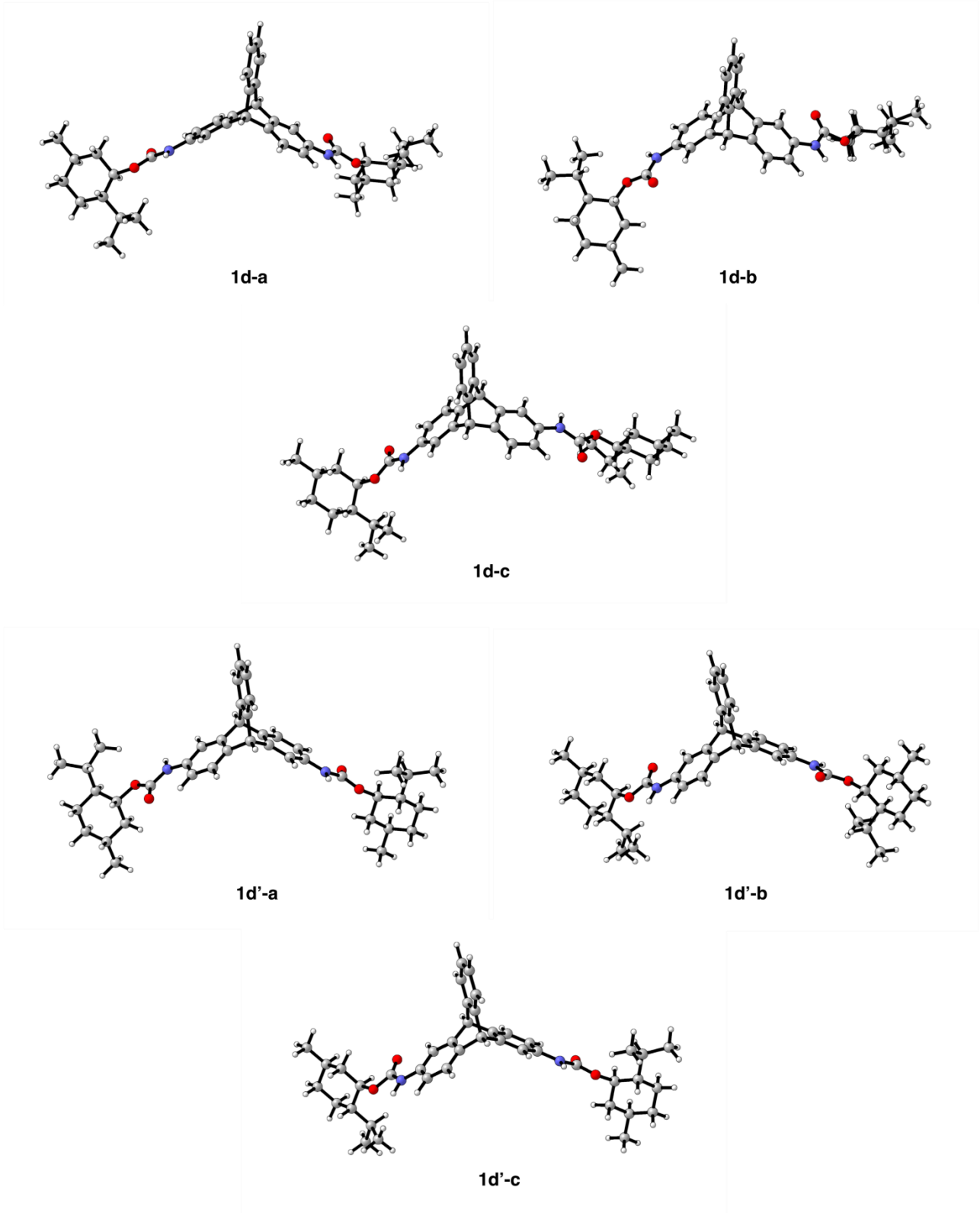

Figure S3. Conformer analysis for diastereomers **1d** and **1d'**. [SMD(DCM)-M06-2X/def2svpp//B3LYP/6-31g(d)]

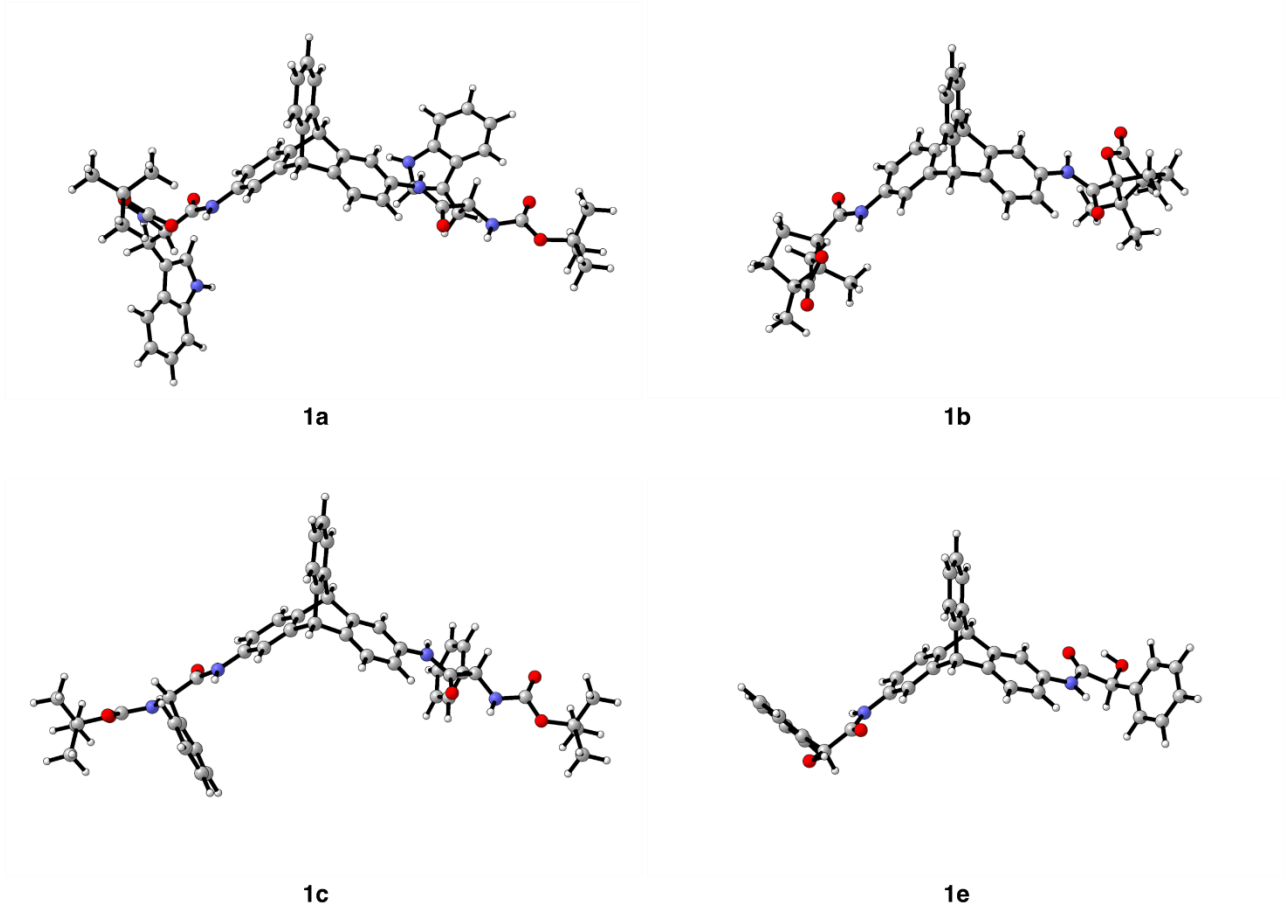

Figure S4. Most stable conformers for **1a**, **1b**, **1c** and **1e**. [SMD(DCM)-M06-2X/def2svpp//B3LYP/6-31g(d)]

Table S2. Boltzmann population analysis, dipole moment and polarizability for conformers of **1d**

	ΔΔG (kcal mol^{-1})	Boltzmann population	Dipole (Debye)	Polarizability (α)	Dipole weighted (Debye)	Polarizability weighted (α)
1-d-a	0.0	**61.9**	4.70	617.43		
1-d-b	0.2	**22.9**	2.89	616.61	3.59	617.31
1-d-c	0.4	**15.2**	0.09	617.90		
1-d'-a	0.1	**28.9**	0.48	618.10		
1-d'-b	0.2	**24.6**	2.45	616.68	3.00	617.33
1-d'-c	0.2	**46.5**	4.85	617.19		

Cartesian coordinates

1a
B3LYP/6-31g(d),
el. energy = -2792.857776 a.u.

C	0.22386300	-2.61088200	1.38925400
C	-0.85931600	-2.82462700	-0.96174000
H	-1.31425300	-2.91474200	-1.95154900
H	0.67933700	-2.52223300	2.37924500
C	1.10555700	-2.04552500	0.27337800
C	0.51884100	-2.16142400	-0.99861000
C	2.35467700	-1.46701700	0.42130100
C	1.20062000	-1.69410600	-2.11322800
C	3.04481500	-0.99145300	-0.71215400
H	2.80754300	-1.37796600	1.40737600
C	2.46539600	-1.10732700	-1.98189900
H	0.75759600	-1.77928600	-3.10273100
H	3.00018200	-0.74164800	-2.84672900
C	-1.69877300	-1.98842000	0.00740200
C	-1.11150300	-1.87238800	1.27917300
C	-2.91267300	-1.38152600	-0.26565300
C	-1.75679400	-1.14272900	2.26762200
C	-3.56727600	-0.63975300	0.73935500
H	-3.36748900	-1.47334400	-1.25006000
C	-2.98483200	-0.52174400	2.00852400
H	-1.31438400	-1.04902900	3.25702900
H	-3.49485100	0.04368500	2.77536000
C	-0.06514900	-4.06206900	0.99648900
C	-0.65409200	-4.17741800	-0.27521500
C	0.19305600	-5.19680400	1.75527300
C	-0.98276600	-5.42745900	-0.78460700
C	-0.13887600	-6.45793800	1.24169200
H	0.64868000	-5.10811700	2.73889400
C	-0.72229000	-6.57242100	-0.01933700
H	-1.43703600	-5.51723200	-1.76872100
H	0.06107000	-7.34917300	1.83055400
H	-0.97645800	-7.55297400	-0.41302000
N	4.31542300	-0.41598500	-0.48330600
H	4.58645000	-0.34155800	0.49128700
N	-4.79606500	-0.04343500	0.38626500
H	-5.14129000	-0.25976900	-0.54870800
C	5.18287500	0.14451000	-1.37653100
C	-5.67326200	0.64933800	1.17483200
O	-5.50351800	0.91448300	2.36086500
O	4.99174600	0.21870300	-2.58750100
C	-6.96464500	1.05564900	0.41256100
H	-6.68630700	1.42821700	-0.57807600
C	6.47059700	0.69994300	-0.73362900
H	6.96513500	-0.10499900	-0.17521200
N	-7.81314000	-0.11798100	0.19499000
H	-8.52491600	-0.34706500	0.87501700
N	7.32569600	1.11743200	-1.82288500
H	6.92009000	1.06848500	-2.75088700
C	8.67551400	1.19611300	-1.66933600
C	-7.62822600	-0.97187200	-0.84890500
O	-6.71769800	-0.85614100	-1.66876500
O	9.25233900	1.07664000	-0.59385200
O	-8.57912000	-1.92678700	-0.84183100
O	9.25901500	1.43924600	-2.86702900
C	10.71497700	1.60623400	-2.98441500
C	-8.59383300	-3.00831100	-1.84628300
C	-7.31039300	-3.83811400	-1.74308200
H	-7.38401500	-4.70901700	-2.40391600
H	-6.43690900	-3.25229600	-2.03323100
H	-7.17093700	-4.20035400	-0.71871400
C	-8.79813600	-2.41690600	-3.24442800
H	-7.94374300	-1.80740100	-3.54278700
H	-8.92381800	-3.22782300	-3.97063200
H	-9.70151600	-1.79764100	-3.26756900
C	-9.81049700	-3.83355600	-1.42018900
H	-9.68124900	-4.21793600	-0.40328600
H	-10.71981200	-3.22452700	-1.44686400
H	-9.94257500	-4.68342700	-2.09774400
C	10.89806100	1.86433600	-4.48256000
H	10.52677600	1.01738700	-5.06860600
H	10.35117600	2.76167400	-4.78972100
H	11.95900200	2.00793400	-4.71304400
C	11.17447600	2.81739300	-2.16522200
H	11.02683200	2.64748400	-1.09763300
H	12.23848100	3.00452700	-2.34968900
H	10.61567100	3.71147200	-2.46334700
C	11.42854200	0.31611100	-2.56528600
H	12.50224400	0.40715200	-2.76546000
H	11.28382100	0.11590700	-1.50260900
H	11.04628400	-0.53349800	-3.14192600
C	6.19596200	1.87449000	0.26186700
H	7.14568600	2.41288200	0.34711600
H	5.47407300	2.56516100	-0.18970700
C	-7.74136200	2.14319900	1.17458700
H	-8.74627300	2.20034500	0.73905800
H	-7.84844900	1.82229100	2.21640800
C	-7.08922700	3.49596100	1.11214300
C	-7.34208300	4.52725700	0.13387400
C	-6.12438900	3.98883400	1.95593700
C	-6.49471300	5.62547000	0.45112200
C	-8.20238400	4.63725700	-0.97294000
H	-5.65218200	3.50862100	2.80068800
N	-5.76702000	5.26501800	1.56706800
C	-6.48762900	6.80657100	-0.29766200
C	-8.19839600	5.80816500	-1.72069000
H	-8.86310600	3.81686600	-1.24322500
H	-5.07215400	5.83620300	2.02166500
C	-7.34841400	6.88244200	-1.38678600
H	-5.83308900	7.63530700	-0.03946800
H	-8.85931400	5.90057400	-2.57828200
H	-7.36666700	7.78586100	-1.99022000
C	5.74719900	1.45213900	1.63196800
C	6.55660000	0.78277700	2.62781500
C	4.51229400	1.64583200	2.20635400
C	5.74381100	0.60036600	3.77916900
C	7.89157400	0.33712600	2.65220800
H	3.63164000	2.12445500	1.79881200

N	4.50002200	1.12917600	3.48912100
C	6.22139400	-0.01604700	4.94079200
C	8.36727300	-0.27409500	3.80557200
H	8.53368200	0.47639300	1.78607700
H	3.72739200	1.19498900	4.13322000
C	7.54191100	-0.45009200	4.93583100
H	5.58770400	-0.14823300	5.81408700
H	9.39580300	-0.62242400	3.84136800
H	7.94618600	-0.93180900	5.82201800

1b

B3LYP/6-31g(d),

el. energy = -2109.285877 a.u.

C	-0.50594500	2.65512200	1.19631000
C	0.50596700	2.65512100	-1.19634300
H	0.93087700	2.65532700	-2.20345900
H	-0.93085500	2.65532500	2.20342600
C	-1.39777100	1.95022000	0.17178300
C	-0.84918800	1.94894500	-1.12241400
C	-2.62276900	1.35332300	0.41626100
C	-1.54201300	1.34394200	-2.16160200
C	-3.32415100	0.73951700	-0.64045800
H	-3.04593800	1.35548000	1.41934000
C	-2.78181400	0.73507200	-1.93174600
H	-1.12755100	1.33747500	-3.16696500
H	-3.32720100	0.26268300	-2.73642600
C	1.39779600	1.95022500	-0.17181400
C	0.84921000	1.94895000	1.12238200
C	2.62279900	1.35333600	-0.41629000
C	1.54203100	1.34394500	2.16157100
C	3.32417300	0.73952200	0.64042900
H	3.04598000	1.35551300	-1.41936400
C	2.78183100	0.73506900	1.93171500
H	1.12757000	1.33748000	3.16693400
H	3.32722000	0.26268700	2.73639700
C	-0.27488300	4.06537200	0.64699500
C	0.27489600	4.06537100	-0.64703100
C	-0.54911700	5.26460800	1.29261300
C	0.54912300	5.26460600	-1.29265400
C	-0.27244800	6.47451700	0.64164500
H	-0.97390000	5.26515600	2.29379500
C	0.27244400	6.47451600	-0.64169100
H	0.97390600	5.26515400	-2.29383500
H	-0.48450200	7.41585300	1.14149000
H	0.48449200	7.41585200	-1.14154000
N	-4.56677600	0.14942700	-0.31972100
H	-4.86543800	0.23012600	0.64530700
N	4.56678700	0.14940600	0.31969100
H	4.86535200	0.22991300	-0.64538300
C	-5.44662100	-0.49929400	-1.13618800
C	5.44673600	-0.49912300	1.13620300
C	6.69532100	-1.02197800	0.43981500
C	6.85488800	-2.57616200	0.33847000
C	8.03866000	-0.54275600	1.02533100
C	7.59438900	-1.46974800	-1.61436200
C	8.13855600	-2.42271500	-0.55391600
C	9.04825800	-1.49698200	0.32532900
H	8.03759900	-0.63725200	2.11292400
H	8.19968700	0.50915400	0.77439500
H	9.60898100	-2.10310200	1.04319000
H	9.78007700	-0.96394000	-0.28929000
C	-6.69526300	-1.02204100	-0.43982000
C	-6.85493000	-2.57620100	-0.33837300
C	-8.03854500	-0.54279000	-1.02544800
C	-7.59447800	-1.46959300	1.61433900
C	-8.13863000	-2.42261800	0.55393900
C	-9.04823700	-1.49690500	-0.32542800
H	-8.03742600	-0.63737000	-2.11303300
H	-8.19952800	0.50914900	-0.77460100
H	-9.60895100	-2.10305300	-1.04327200
H	-9.78006100	-0.96377400	0.28910900
O	5.30402400	-0.69735100	2.33971700
O	-5.30381000	-0.69771100	-2.33966000
O	-6.72032500	-0.61764300	0.96959300
O	6.72033200	-0.61768900	-0.96962700
O	-7.83844000	-1.37751000	2.78742500
O	7.83830600	-1.37775500	-2.78746300
C	-5.67506000	-3.25369900	0.38026100
H	-5.90260700	-4.30831600	0.56951800
H	-4.77863700	-3.22065300	-0.24885100
H	-5.42946600	-2.78836700	1.33931300
C	-7.07594200	-3.28560900	-1.68128300
H	-6.19556700	-3.16163700	-2.31794100
H	-7.22860800	-4.35755600	-1.51132800
H	-7.93674200	-2.91148300	-2.23968300
C	-8.81360000	-3.65695800	1.12349000
H	-8.11893400	-4.25379700	1.72321600
H	-9.64320800	-3.36878000	1.77727600
H	-9.21098800	-4.28920700	0.32207500
C	7.07592200	-3.28549700	1.68141600
H	6.19558800	-3.16142900	2.31810800
H	7.22851800	-4.35746500	1.51152400
H	7.93677500	-2.91139200	2.23974800
C	5.67494500	-3.25363400	-0.38006500
H	5.90242600	-4.30827300	-0.56927700
H	4.77855700	-3.22050400	0.24909000
H	5.42932900	-2.78834100	-1.33913200
C	8.81343300	-3.65713400	-1.12340500
H	8.11871800	-4.25395700	-1.72308900
H	9.64305400	-3.36905100	-1.77721600
H	9.21078600	-4.28936300	-0.32195600

1c

B3LYP/6-31g(d),

el. energy = -2451.080504 a.u.

C	0.37173100	3.08679100	-1.24450100
C	-0.37167100	3.08679700	1.24453200
H	-0.68330700	3.08694000	2.29227600
H	0.68336700	3.08693000	-2.29224500
C	1.37051500	2.38193200	-0.32386100
C	0.96730900	2.38092600	1.02247900
C	2.56135500	1.78479800	-0.70095500
C	1.77015000	1.77593000	1.97903600
C	3.37454300	1.17078300	0.27205500
H	2.87075500	1.78704600	-1.74487200
C	2.97729400	1.16711900	1.61477700
H	1.46853400	1.76845000	3.02377600
H	3.60378900	0.69100900	2.35538900
C	-1.37038200	2.38180300	0.32391500
C	-0.96717400	2.38078700	-1.02242500
C	-2.56116200	1.78456000	0.70102800
C	-1.76995000	1.77567300	-1.97896400

C	-3.37428400	1.17043100	-0.27196500
H	-2.87056700	1.78681400	1.74494300
C	-2.97702900	1.16674900	-1.61468500
H	-1.46832700	1.76818200	-3.02370100
H	-3.60347600	0.69053600	-2.35527400
C	0.20222600	4.49712000	-0.67328900
C	-0.20231600	4.49712200	0.67327200
C	0.40356500	5.69637400	-1.34514200
C	-0.40378100	5.69637700	1.34508600
C	0.19998600	6.90632400	-0.66780000
H	0.71546700	5.69699600	-2.38704500
C	-0.20032900	6.90632600	0.66770300
H	-0.71568300	5.69700100	2.38698900
H	0.35555500	7.84766500	-1.18795900
H	-0.35599700	7.84766800	1.18783100
N	4.57943900	0.58788600	-0.18335100
H	4.73274000	0.63638500	-1.18373300
N	-4.57910600	0.58739800	0.18344600
H	-4.73238500	0.63578300	1.18383700
C	5.51762400	-0.11150300	0.51746100
C	-5.51744800	-0.11166800	-0.51746900
O	-5.45739400	-0.36730900	-1.71531500
O	5.45750300	-0.36742900	1.71523700
C	-6.74508200	-0.54340000	0.33326900
H	-7.32034000	0.36824200	0.55309500
C	-6.34224900	-1.16713400	1.66516000
C	-6.54716600	-0.47086800	2.86115400
C	-5.73170100	-2.42792000	1.70733500
C	-6.13830100	-1.01712700	4.08110200
H	-7.05573300	0.49066100	2.84110400
C	-5.32807000	-2.97534800	2.92310000
H	-5.58692500	-2.98125200	0.78331200
C	-5.52630600	-2.26941400	4.11380800
H	-6.31323600	-0.46939100	5.00324200
H	-4.85744900	-3.95470300	2.94361200
H	-5.21217900	-2.69924800	5.06106100
C	6.74519300	-0.54327500	-0.33335600
H	7.32045500	0.36833100	-0.55330900
C	6.34216300	-1.16708800	-1.66515600
C	6.54690100	-0.47087600	-2.86121700
C	5.73161100	-2.42787200	-1.70718400
C	6.13785100	-1.01718300	-4.08107500
H	7.05548300	0.49065000	-2.84129000
C	5.32779400	-2.97535200	-2.92286800
H	5.58697200	-2.98117000	-0.78312000
C	5.52584400	-2.26947400	-4.11363400
H	6.31265000	-0.46949300	-5.00326800
H	4.85716600	-3.95470700	-2.94325400
H	5.21157200	-2.69934300	-5.06082200
N	-7.53520600	-1.42164900	-0.50205800
H	-7.18347800	-1.54835400	-1.44574600
N	7.53533100	-1.42145200	0.50198800
H	7.18350000	-1.54848100	1.44558500
C	8.88458800	-1.52554500	0.28583600
C	-8.88450700	-1.52549600	-0.28596100
O	-9.45260400	-1.07536400	0.69662800
O	9.45276800	-1.07539300	-0.69668900
O	-9.45180800	-2.20613600	-1.30996500
O	9.45177400	-2.20645700	1.30974000
C	10.89359400	-2.49552600	1.31997200
C	-10.89360800	-2.49540900	-1.32004100
C	-11.69297100	-1.18793700	-1.35067400
H	-12.75867700	-1.41073000	-1.47636000
H	-11.55783600	-0.62412700	-0.42642800
H	-11.37392500	-0.56739000	-2.19550200
C	-11.26147900	-3.37348200	-0.11904500
H	-11.11641300	-2.83519000	0.81886100
H	-12.31158800	-3.67828100	-0.19357000
H	-10.64453900	-4.27881400	-0.10755300
C	-11.06718800	-3.26751100	-2.63073000
H	-10.76030900	-2.65416800	-3.48418400
H	-10.46031700	-4.17872300	-2.62554700
H	-12.11673400	-3.54972900	-2.76537000
C	11.06713900	-3.26771500	2.63061900
H	10.76016600	-2.65445800	3.48410200
H	10.46032000	-4.17896200	2.62532400
H	12.11669100	-3.54988300	2.76530700
C	11.26169000	-3.37345000	0.11893100
H	11.11656100	-2.83510300	-0.81893600
H	12.31185200	-3.67806100	0.19346800
H	10.64491100	-4.27889000	0.10734100
C	11.69281200	-1.18797000	1.35079200
H	12.75851500	-1.41066800	1.47666400
H	11.55779500	-0.62412300	0.42655100
H	11.37355700	-0.56748900	2.19559000

1e

B3LYP/6-31g(d),

el. energy = -1799.131574 a.u.

C	-0.34508600	1.57702300	1.25158200
C	0.34509900	1.57648200	-1.25201100
H	0.63574900	1.57508800	-2.30542400
H	-0.63573300	1.57608500	2.30499600
C	-1.36463000	0.87094200	0.35409300
C	-0.98848200	0.87139100	-0.99928600
C	-2.54588200	0.27946300	0.77927700
C	-1.81217000	0.26790400	-1.94040800
C	-3.37610100	-0.33084800	-0.17918200
H	-2.83902300	0.28344800	1.82045500
C	-3.00489200	-0.33272600	-1.52989600
H	-1.53778700	0.25819000	-2.99227100
H	-3.65099800	-0.80623500	-2.26609600
C	1.36463400	0.87076900	-0.35421800
C	0.98848900	0.87180700	0.99916000
C	2.54587700	0.27909100	-0.77915300
C	1.81217500	0.26872100	1.94054200
C	3.37608100	-0.33083100	0.17956600
H	2.83901500	0.28261200	-1.82033200
C	3.00488000	-0.33211400	1.53028400
H	1.53779800	0.25947300	2.99241000
H	3.65098200	-0.80531400	2.26668600
C	-0.18819700	2.98734400	0.67665900
C	0.18823300	2.98705100	-0.67769200
C	-0.37698500	4.18648800	1.35238200
C	0.37703800	4.18590400	-1.35392700
C	-0.18722100	5.39611200	0.67050200
H	-0.66972700	4.18696300	2.39975200
C	0.18729400	5.39582300	-0.67256300
H	0.66977500	4.18592700	-2.40129900
H	-0.33332400	6.33761600	1.19316100
H	0.33341400	6.33710000	-1.19562400
N	-4.59502500	-0.96735300	0.15574100

H	-5.11974500	-1.33834500	-0.62802500
N	4.59502100	-0.96745700	-0.15507500
H	5.11989000	-1.33784100	0.62887900
C	-5.20543200	-1.07859000	1.36440000
C	5.20512200	-1.07978100	-1.36378400
O	4.79040900	-0.60981100	-2.42210800
O	-4.79096700	-0.60769400	2.42240700
C	6.50555500	-1.93832200	-1.39720800
H	6.16729600	-2.99017500	-1.35132500
C	7.42818900	-1.68187300	-0.22031500
C	7.39734800	-2.51564100	0.90445500
C	8.30124400	-0.58643400	-0.23289200
C	8.20890200	-2.24822900	2.01078300
H	6.75322800	-3.39366100	0.90698900
C	9.11563300	-0.32417500	0.86681300
H	8.34508800	0.03888400	-1.11884700
C	9.06812500	-1.14998000	1.99426000
H	8.17942100	-2.90719100	2.87446900
H	9.79224300	0.52606000	0.84525000
H	9.70581000	-0.94312700	2.84940000
C	-6.50587000	-1.93709900	1.39826200
H	-6.16760900	-2.98899500	1.35343100
C	-7.42818800	-1.68172000	0.22088700
C	-7.39701200	-2.51647900	-0.90313200
C	-8.30126700	-0.58627900	0.23225000
C	-8.20826300	-2.25006100	-2.00992700
H	-6.75287800	-3.39449100	-0.90471300
C	-9.11535000	-0.32501200	-0.86791400
H	-8.34537000	0.03980900	1.11764800
C	-9.06750600	-1.15181400	-1.99462000
H	-8.17852000	-2.90978800	-2.87302000
H	-9.79198300	0.52522900	-0.84730000
H	-9.70495100	-0.94572200	-2.85012300
O	-7.14991100	-1.67667300	2.61929400
H	-6.46420600	-1.24272600	3.16968100
O	7.14927600	-1.67900600	-2.61864200
H	6.46342300	-1.24557400	-3.16925500

1d-a
B3LYP/6-31g(d),
el. energy = -2042.302472 a.u.

C	-0.36853100	2.89795100	1.23450700
C	0.67358800	2.29051400	-1.06520200
H	1.11240700	2.03441000	-2.03262300
H	-0.80548200	3.15398100	2.20356200
C	-1.28603100	2.02261800	0.37767200
C	-0.72052000	1.69267300	-0.86538400
C	-2.54715900	1.56571600	0.72168500
C	-1.43488400	0.89975000	-1.75242000
C	-3.27109100	0.76180800	-0.18118500
H	-2.98136300	1.82471200	1.68619700
C	-2.71084400	0.42834400	-1.42043800
H	-1.00856100	0.63555000	-2.71731800
H	-3.27028300	-0.18895300	-2.10936000
C	1.51302800	1.79751700	0.11644900
C	0.94609600	2.12560300	1.35899700
C	2.70852300	1.09899700	0.02446700
C	1.59211100	1.74389400	2.52697700
C	3.35954200	0.71352700	1.21162900
H	3.14437900	0.84660200	-0.93302600
C	2.79637300	1.03918200	2.45309000
H	1.17089300	1.98832400	3.49923000
H	3.30291700	0.74068100	3.36860400
C	-0.05190300	4.12894500	0.38110200
C	0.51528800	3.79967500	-0.86276400
C	-0.26739300	5.45767000	0.72465600
C	0.86640500	4.80106300	-1.75947200
C	0.08642000	6.46796400	-0.18017500
H	-0.70592100	5.71237000	1.68693800
C	0.64917600	6.14178900	-1.41329200
H	1.30598700	4.54712300	-2.72122500
H	-0.07936300	7.50934700	0.08285100
H	0.92173900	6.92918100	-2.11101600
N	-4.54827700	0.33153700	0.23421300
H	-4.85406500	0.64081600	1.14666500
N	4.57690700	0.00238600	1.22239400
H	4.95339800	-0.23346300	2.13041200
C	-5.45987000	-0.43109500	-0.45171500
C	5.32071300	-0.43992100	0.15708800
O	5.05991800	-0.29511100	-1.02317900
O	-5.32736200	-0.89401200	-1.56953200
O	-6.55780100	-0.59727800	0.33749700
O	6.42425900	-1.07427000	0.64071100
C	-7.67011100	-1.33414400	-0.23962000
C	-8.42297600	-2.08001000	0.87930900
C	-8.55045000	-0.34393200	-1.00799300
H	-7.24655800	-2.06404200	-0.93780000
C	-9.65132600	-2.75932500	0.22687000
H	-8.80474500	-1.32717100	1.58728200
C	-9.78372000	-1.01823600	-1.62847400
H	-8.87230200	0.44807600	-0.31596200
H	-7.94309500	0.13210700	-1.78665200
C	-10.55048600	-1.77549200	-0.53515200
H	-10.24267400	-3.26363700	0.99725000
H	-9.30908400	-3.54445200	-0.46417300
H	-9.42861300	-1.75831600	-2.36314200
H	-11.39985000	-2.31549700	-0.97435400
H	-10.97703100	-1.04776500	0.17241100
C	7.31831600	-1.66833500	-0.34005100
C	8.76310300	-1.62397000	0.19431400
C	6.82476000	-3.08715000	-0.63792800
H	7.25106800	-1.05999300	-1.24827800
C	9.65268100	-2.35508000	-0.83985500
H	8.79540900	-2.21212400	1.12529700
C	7.72828400	-3.82074400	-1.64120000
H	6.78828800	-3.65049800	0.30600300
H	5.79902800	-3.02751400	-1.02033900
C	9.17847500	-3.78442700	-1.13823300
H	10.68468100	-2.38720200	-0.47725600
H	9.67150200	-1.77807200	-1.77672100
H	7.68982700	-3.26941600	-2.59416800
H	9.84583800	-4.24863100	-1.87649400
H	9.25556700	-4.39261300	-0.22372800
C	-7.50170800	-3.06523800	1.67253100
H	-6.75016200	-3.44914000	0.96587700
C	-6.75671400	-2.35610700	2.81871700
H	-6.17900200	-1.50152200	2.46359200
H	-7.46942700	-1.99362900	3.57175900
H	-6.07175400	-3.04951700	3.32141400
C	-8.23801400	-4.28612700	2.25366800
H	-9.02755400	-3.98371600	2.95395200
H	-8.69392900	-4.91372900	1.48203500

H	-7.53197600	-4.91264600	2.81110400
C	-10.66907700	-0.00704100	-2.36505000
H	-10.11203000	0.50783900	-3.15663100
H	-11.53244800	-0.49986500	-2.82782700
H	-11.05120600	0.75646000	-1.67512300
C	9.23851100	-0.17026100	0.52501400
H	8.73452300	0.50649700	-0.18178500
C	8.84000100	0.25123200	1.95159000
H	9.12481300	1.29326600	2.14050300
H	7.76675300	0.15358000	2.12180200
H	9.35826200	-0.37132100	2.69335600
C	10.75288600	0.05139400	0.35767300
H	11.33121400	-0.60920700	1.01668100
H	11.09516300	-0.11236800	-0.66863700
H	11.00734100	1.08298000	0.62752900
C	7.23913000	-5.24977800	-1.90092000
H	6.21069400	-5.25604700	-2.28075300
H	7.87266600	-5.75726600	-2.63814200
H	7.25800900	-5.84512600	-0.97889600

1d-b

B3LYP/6-31g(d),

el. energy = -2042.302881 a.u.

C	-0.68872400	2.26185000	1.10052400
C	0.68874600	2.26180000	-1.10057400
H	1.26841000	2.26090600	-2.02707200
H	-1.26838800	2.26100100	2.02702300
C	-1.41013100	1.55701100	-0.05132100
C	-0.66163900	1.55660600	-1.23972500
C	-2.66408900	0.96679300	0.01949400
C	-1.18293500	0.95029700	-2.37468800
C	-3.18830700	0.35384900	-1.13412700
H	-3.23983400	0.96840400	0.93547500
C	-2.44368300	0.35025600	-2.32147200
H	-0.61967600	0.93753900	-3.30460500
H	-2.85227600	-0.12425000	-3.21131700
C	1.41020900	1.55713000	0.05134000
C	0.66171800	1.55678100	1.23974500
C	2.66421800	0.96701100	-0.01941800
C	1.18306500	0.95062400	2.37476500
C	3.18848100	0.35421100	1.13425900
H	3.23995400	0.96856400	-0.93540400
C	2.44385700	0.35067000	2.32160400
H	0.61980600	0.93790800	3.30468300
H	2.85248400	-0.12372500	3.21149200
C	-0.37440600	3.67225000	0.59497600
C	0.37431300	3.67222300	-0.59516200
C	-0.74884200	4.87154900	1.18794500
C	0.74865200	4.87149600	-1.18824400
C	-0.37192900	6.08164800	0.58947900
H	-1.32939300	4.87168400	2.10763400
C	0.37164100	6.08162200	-0.58989300
H	1.32920300	4.87159100	-2.10793300
H	-0.66179700	7.02307200	1.04869200
H	0.66143400	7.02302500	-1.04919500
N	-4.45228200	-0.27112800	-1.16366000
H	-4.72807000	-0.68852100	-2.04206600
N	4.45252800	-0.27061300	1.16386400
H	4.72840900	-0.68779100	2.04234400
C	-5.36556100	-0.40636900	-0.14877700
C	5.36559400	-0.40635100	0.14885200
O	5.24876800	-0.00538800	-0.99485900
O	-5.24894500	-0.00491000	0.99478100
O	-6.45065700	-1.07028000	-0.63553100
O	6.45076300	-1.07006800	0.63569900
C	-7.51819700	-1.35632900	0.30874000
C	-8.86838000	-1.36003600	-0.43424100
C	-7.20293000	-2.68638500	0.99938600
H	-7.51733900	-0.55064200	1.05067300
C	-9.95214300	-1.76284400	0.59456600
H	-8.83070900	-2.15531100	-1.19570300
C	-8.29628900	-3.09880400	1.99717700
H	-7.09416000	-3.46377600	0.22895600
H	-6.23609600	-2.59566200	1.50812800
C	-9.65725900	-3.10128200	1.28644100
H	-10.92514800	-1.82219800	0.09727500
H	-10.04178300	-0.97440000	1.35704200
H	-8.33343800	-2.33488600	2.79006700
H	-10.45698600	-3.33097000	2.00309600
H	-9.66893300	-3.90888800	0.53825100
C	7.51811500	-1.35662900	-0.30863400
C	8.86851200	-1.35964300	0.43397100
C	7.20274000	-2.68722600	-0.99819900
H	7.51694500	-0.55148900	-1.05115600
C	9.95200600	-1.76333400	-0.59479200
H	8.83107900	-2.15422000	1.19617600
C	8.29583400	-3.10040000	-1.99595600
H	7.09418500	-3.46402900	-0.22714600
H	6.23575900	-2.59691400	-1.50674400
C	9.65696300	-3.10231900	-1.28553100
H	10.92512800	-1.82231300	-0.09769200
H	10.04148000	-0.97549700	-1.35791700
H	8.33278900	-2.33709000	-2.78944100
H	10.45653400	-3.33257200	-2.00217900
H	9.66880300	-3.90933000	-0.53670400
C	-9.15771900	-0.00648100	-1.16439700
H	-8.69003400	0.79214000	-0.56856400
C	-8.53664200	0.02695300	-2.57314800
H	-7.46453500	-0.17421900	-2.55160900
H	-9.00940100	-0.72632800	-3.21769800
H	-8.69370500	1.00587700	-3.04184200
C	-10.65332900	0.33858200	-1.28380400
H	-11.19903400	-0.42816300	-1.84899700
H	-11.14177600	0.45220900	-0.31128600
H	-10.77212200	1.28556300	-1.82312300
C	-7.98150500	-4.44744900	2.65368800
H	-7.01781100	-4.42108000	3.17585400
H	-8.75201500	-4.72178400	3.38410100
H	-7.93291900	-5.24763100	1.90384000
C	9.15814400	-0.00543200	1.16278200
H	8.69082200	0.79272100	0.56603100
C	8.53692900	0.02974000	2.57143300
H	8.69453500	1.00903600	3.03916600
H	7.46471000	-0.17080800	2.55001200
H	9.00918500	-0.72317700	3.21677700
C	10.65386900	0.33920600	1.28202900
H	11.19923300	-0.42723700	1.84796400
H	11.14245300	0.45178400	0.30946100
H	10.77295400	1.28662600	1.82051200
C	7.98089200	-4.44954900	-2.65135200
H	7.01707600	-4.42358200	-3.17331300
H	8.75122900	-4.72445000	-3.38173400

H	7.93248100	-5.24915200	-1.90087500

1d-c

B3LYP/6-31g(d),

el. energy = -2042.302338 a.u.

C	-0.35183200	2.79262800	1.24999100
C	0.35183000	2.79264600	-1.25001600
H	0.64662500	2.79317000	-2.30275100
H	-0.64662400	2.79312900	2.30272700
C	-1.36563400	2.08791400	0.34552200
C	-0.98383400	2.08714500	-1.00667300
C	-2.54976400	1.49001800	0.74271500
C	-1.80333600	1.48161400	-1.94865500
C	-3.37990500	0.87454200	-0.21535300
H	-2.84115700	1.49207400	1.79190900
C	-3.00364900	0.87190600	-1.56421700
H	-1.52012900	1.47437200	-2.99870400
H	-3.64455900	0.39925900	-2.29527000
C	1.36550400	2.08768400	-0.34559500
C	0.98370800	2.08690500	1.00660000
C	2.54952800	1.48959800	-0.74282100
C	1.80309800	1.48117200	1.94854800
C	3.37954400	0.87389500	0.21520700
H	2.84093900	1.49169200	-1.79201000
C	3.00328200	0.87123600	1.56407000
H	1.51988600	1.47391900	2.99859600
H	3.64410000	0.39842000	2.29509500
C	-0.19187500	4.20296400	0.67645200
C	0.19212400	4.20297300	-0.67638100
C	-0.38292000	5.40238700	1.35091300
C	0.38337500	5.40240600	-1.35076700
C	-0.18964900	6.61259800	0.67078100
H	-0.67895300	5.40293100	2.39749800
C	0.19031500	6.61260800	-0.67055800
H	0.67940600	5.40296400	-2.39735300
H	-0.33728300	7.55394600	1.19340000
H	0.33811100	7.55396200	-1.19311800
N	-4.56775300	0.28196500	0.25959700
H	-4.73804300	0.34563600	1.25394900
N	4.56722900	0.28102800	-0.25979600
H	4.73726200	0.34426700	-1.25421900
C	-5.54725400	-0.36301600	-0.45348000
C	5.54711000	-0.36328100	0.45337400
O	5.57266000	-0.54165400	1.65711000
O	-5.57252100	-0.54190600	-1.65714400
O	-6.50288600	-0.78579400	0.41977800
O	6.50270000	-0.78613100	-0.41988700
C	-7.66212800	-1.45130100	-0.15205400
C	-8.18770100	-2.50511500	0.84212900
C	-8.69855000	-0.38106800	-0.50681900
H	-7.32778100	-1.95328100	-1.06620100
C	-9.47491200	-3.10684200	0.22832500
H	-8.48145600	-1.97983700	1.76490900
C	-9.98671900	-0.98528800	-1.08694000
H	-8.93628300	0.19095800	0.40201200
H	-8.24860200	0.31779900	-1.22179500
C	-10.52924100	-2.04645800	-0.11903300
H	-9.90910100	-3.83030600	0.92513200
H	-9.21597300	-3.66985900	-0.68108400
H	-9.72560100	-1.49286700	-2.02915800
H	-11.41459500	-2.53283500	-0.54972000
H	-10.86551600	-1.55021800	0.80445800
C	7.66210400	-1.45133400	0.15199900
C	8.18779800	-2.50525100	-0.84199800
C	8.69835700	-0.38084600	0.50650500
H	7.32790800	-1.95320100	1.06626600
C	9.47514400	-3.10662700	-0.22810900
H	8.48143200	-1.98013200	-1.76491000
C	9.98663800	-0.98472500	1.08672300
H	8.93596800	0.19102700	-0.40245400
H	8.24830000	0.31808500	1.22134400
C	10.52930700	-2.04600500	0.11902000
H	9.90944800	-3.83014300	-0.92479000
H	9.21631700	-3.66952200	0.68140800
H	9.72562400	-1.49215100	2.02905300
H	11.41474500	-2.53216300	0.54978100
H	10.86548200	-1.54989700	-0.80457900
C	-7.10624500	-3.57204000	1.21735200
H	-6.46254900	-3.70843500	0.33493400
C	-6.21838600	-3.10158900	2.38440300
H	-5.74561000	-2.14049100	2.17687500
H	-6.81529800	-2.99434200	3.30014000
H	-5.42981300	-3.83536800	2.59013200
C	-7.68254800	-4.95500400	1.57184400
H	-8.36034800	-4.89915500	2.43361800
H	-8.22933400	-5.41245200	0.74178500
H	-6.86779900	-5.63640500	1.84309100
C	-11.02477100	0.09672400	-1.40402800
H	-10.62888000	0.83300100	-2.11339300
H	-11.93002800	-0.33958200	-1.84285300
H	-11.32131300	0.63531900	-0.49468200
C	7.10655200	-3.57247500	-1.21695700
H	6.46306100	-3.70899300	-0.33440400
C	6.21833500	-3.10235900	-2.38386600
H	5.42991600	-3.83636800	-2.58936400
H	5.74535200	-2.14136800	-2.17633100
H	6.81503400	-2.99504400	-3.29973400
C	7.68315800	-4.95530600	-1.57148200
H	8.36083600	-4.89929600	-2.43334200
H	8.23016000	-5.41260000	-0.74148200
H	6.86854600	-5.63691600	-1.84261700
C	11.02452000	0.09751900	1.40356300
H	10.62852700	0.83387300	2.11279000
H	11.92986000	-0.33855200	1.84245200
H	11.32095400	0.63598000	0.49410200

1d'-a

B3LYP/6-31g(d),

el. energy = -2042.302321 a.u.

C	0.37216400	2.66625300	1.24394400
C	-0.37217700	2.66627200	-1.24426800
H	-0.68408700	2.66682600	-2.29205900
H	0.68407400	2.66679200	2.29173500
C	1.37107500	1.96154800	0.32309300
C	0.96722300	1.96071600	-1.02268400
C	2.56192900	1.36436700	0.70081400
C	1.77171700	1.35600100	-1.97802100
C	3.37686300	0.74982200	-0.27080900
H	2.87077300	1.36715000	1.74500300
C	2.97900200	0.74785300	-1.61346700
H	1.47152600	1.34893800	-3.02334600
H	3.60784500	0.27512600	-2.35485900

C	-1.37122600	1.96180100	-0.32338300
C	-0.96736800	1.96093800	1.02239200
C	-2.56219800	1.36483900	-0.70107600
C	-1.77197200	1.35641600	1.97776000
C	-3.37723000	0.75047500	0.27057900
H	-2.87105800	1.36765800	-1.74526000
C	-2.97937600	0.74849100	1.61323400
H	-1.47178000	1.34933700	3.02308500
H	-3.60831600	0.27591400	2.35464600
C	0.20315000	4.07663300	0.67299400
C	-0.20290000	4.07664400	-0.67337900
C	0.40545300	5.27603900	1.34418500
C	-0.40497900	5.27606000	-1.34461900
C	0.20129500	6.48624100	0.66722500
H	0.71861400	5.27658300	2.38577000
C	-0.20059500	6.48625200	-0.66770700
H	-0.71813900	5.27662200	-2.38620400
H	0.35765200	7.42758700	1.18729900
H	-0.35677900	7.42760500	-1.18782000
N	4.57516100	0.16226800	0.18382100
H	4.75860800	0.22048100	1.17616900
N	-4.57568500	0.16318200	-0.18395600
H	-4.75896400	0.22098000	-1.17636000
C	5.52469400	-0.51490500	-0.53987400
C	-5.52489500	-0.51442000	0.53975500
O	-5.50793500	-0.73270900	1.73706200
O	5.50786900	-0.73324000	-1.73717600
O	-6.51296200	-0.90549900	-0.31191200
C	-7.59159300	-1.69578400	0.25897800
C	-8.89831300	-1.40261500	-0.50366100
C	-7.17888200	-3.16985300	0.21127900
H	-7.70467900	-1.38172200	1.30207900
C	-9.98373500	-2.34092800	0.07711700
H	-8.74593200	-1.69253400	-1.55554700
C	-9.28785800	0.11254900	-0.47220600
C	-8.27164700	-4.10014500	0.76023100
H	-6.95658500	-3.43751900	-0.83210600
H	-6.25111000	-3.29175500	0.78251800
C	-9.58980200	-3.82374900	0.02318700
H	-10.92123200	-2.19826500	-0.46901400
H	-10.18775900	-2.05943200	1.12125000
H	-8.93765300	0.51954400	0.48869100
C	-8.60152400	0.90386300	-1.60110300
C	-10.80313500	0.37487000	-0.54654100
H	-8.42279500	-3.85124000	1.82268400
C	-7.85517000	-5.57253100	0.67357400
H	-10.39597600	-4.43597200	0.44882500
H	-9.48458800	-4.13518000	-1.02756900
H	-8.83801800	1.97187100	-1.52321800
H	-7.51661800	0.79108200	-1.57824400
H	-8.95711600	0.55860800	-2.58127900
H	-11.23578100	-0.02755900	-1.47176900
H	-11.35052300	-0.05625600	0.29708900
H	-10.99189400	1.45471800	-0.54258000
H	-6.92492400	-5.75648300	1.22387300
H	-8.62829000	-6.22797900	1.09202800
H	-7.69120300	-5.87381900	-0.36914500
O	6.51288900	-0.90555700	0.31183700
C	7.59175200	-1.69560100	-0.25894500
C	8.89822800	-1.40248300	0.50414400
C	7.17915400	-3.16972100	-0.21168900
H	7.70510500	-1.38129100	-1.30194400
C	9.98388700	-2.34064800	-0.07645500
H	8.74552900	-1.69257900	1.55593600
C	9.28780500	0.11268400	0.47306000
C	8.27214000	-4.09980500	-0.76053700
H	6.95659500	-3.43763200	0.83157800
H	6.25155400	-3.29156800	-0.78321400
C	9.59003100	-3.82350400	-0.02300000
H	10.92118400	-2.19806400	0.47003500
H	10.18825700	-2.05890300	-1.12045300
H	8.93822900	0.51973900	-0.48804300
C	8.60081600	0.90400900	1.60155500
C	10.80304700	0.37497200	0.54838400
H	8.42360600	-3.85062800	-1.82288200
C	7.85571800	-5.57223500	-0.67437600
H	10.39639100	-4.43557000	-0.44851200
H	9.48449100	-4.13518900	1.02764900
H	8.83757700	1.97197700	1.52392500
H	7.51590800	0.79145100	1.57794500
H	8.95566700	0.55860000	2.58194500
H	11.23509000	-0.02758600	1.47383800
H	11.35097600	-0.05604500	-0.29494900
H	10.99182700	1.45481700	0.54468600
H	6.92565600	-5.75610400	-1.22501400
H	8.62900800	-6.22753400	-1.09274700
H	7.69143800	-5.87379100	0.36821800

1d'-b

B3LYP/6-31g(d),

el. energy = -2042.302917 a.u.

C	-0.71574900	2.39247700	-1.08333200
C	0.71569500	2.39262100	1.08304700
H	1.31816000	2.39177900	1.99488200
H	-1.31821300	2.39151200	-1.99516700
C	-1.40842700	1.68777800	0.08614200
C	-0.63113200	1.68820200	1.25589600
C	-2.66357500	1.09717600	0.04636100
C	-1.12500800	1.08379600	2.40405900
C	-3.16023200	0.48674900	1.21344800
H	-3.26157200	1.09819000	-0.85524100
C	-2.38706500	0.48454600	2.38239700
H	-0.53917600	1.07172000	3.31992800
H	-2.77370500	0.01056800	3.28227400
C	1.40831200	1.68763700	-0.08629000
C	0.63102000	1.68791300	-1.25604700
C	2.66339600	1.09691100	-0.04638300
C	1.12485200	1.08324900	-2.40409300
C	3.16001200	0.48623100	-1.21335600
H	3.26138100	1.09803100	0.85522700
C	2.38686000	0.48389700	-2.38231400
H	0.53903000	1.07105600	-3.31996800
H	2.77347100	0.00973900	-3.28210900
C	-0.38904800	3.80296900	-0.58584000
C	0.38911500	3.80304600	0.58528500
C	-0.77804400	5.00222300	-1.16944700
C	0.77821600	5.00237900	1.16866200
C	-0.38624300	6.21239100	-0.58073200
H	-1.38130600	5.00227500	-2.07440500
C	0.38652000	6.21246700	0.57971400
H	1.38147800	5.00255300	2.07361900
H	-0.68739700	7.15377500	-1.03271400

H	0.68775600	7.15391200	1.03151600
N	-4.42242100	-0.13968600	1.27379300
H	-4.68499000	-0.53942800	2.16438100
N	4.42212400	-0.14037200	-1.27356700
H	4.68454800	-0.54051100	-2.16402000
C	-5.36734500	-0.26003000	0.28640700
C	5.36719700	-0.26027400	-0.28627200
O	5.28690400	0.15915700	0.85395800
O	-5.28693500	0.15899300	-0.85396300
O	-6.43083100	-0.94392700	0.79293300
C	-7.56987700	-1.12591200	-0.09174100
C	-8.27334800	-2.45470800	0.24698900
C	-8.48274900	0.09596600	0.04756400
H	-7.17980400	-1.17531000	-1.11396700
C	-9.52769300	-2.54725500	-0.65504200
H	-8.62522100	-2.39300900	1.28914400
C	-7.31833300	-3.68889100	0.13221300
C	-9.74135700	-0.01377700	-0.82668600
H	-8.77434600	0.19686000	1.10325500
H	-7.91011400	0.99222600	-0.21828600
C	-10.45974700	-1.33506300	-0.51767900
H	-10.08504200	-3.45778600	-0.41459900
H	-9.21445000	-2.64434300	-1.70553900
H	-6.59604100	-3.46898900	-0.66875400
C	-6.52791500	-3.92407000	1.43280100
C	-8.02777400	-5.00094100	-0.24938200
H	-9.41780500	-0.04606400	-1.87924800
C	-10.65890800	1.20114500	-0.65054300
H	-11.32607500	-1.45806400	-1.18119600
H	-10.85719800	-1.29499400	0.50827900
H	-5.82024200	-4.75283400	1.31034700
H	-5.96830100	-3.03829800	1.73690400
H	-7.20942900	-4.19144200	2.25159900
H	-8.78802500	-5.27735200	0.49277200
H	-8.51433100	-4.95143300	-1.22818500
H	-7.29814200	-5.81824200	-0.28670400
H	-10.13729500	2.13345700	-0.89701400
H	-11.54095000	1.12836500	-1.29795800
H	-11.01170200	1.28014100	0.38590700
O	6.43066800	-0.94427100	-0.79268300
C	7.56974400	-1.12601000	0.09201200
C	8.27362100	-2.45452900	-0.24694800
C	8.48228800	0.09614200	-0.04701600
H	7.17963800	-1.17571400	1.11421300
C	9.52791300	-2.54693800	0.65515500
H	8.62555000	-2.39248800	-1.28906200
C	7.31892100	-3.68899700	-0.13253400
C	9.74085800	-0.01343300	0.82731500
H	8.77394500	0.19728200	-1.10266700
H	7.90940200	0.99220000	0.21895200
C	10.45964800	-1.33445900	0.51811700
H	10.08552700	-3.45727000	0.41456500
H	9.21462300	-2.64433100	1.70561100
H	6.59634700	-3.46935500	0.66825000
C	6.52893200	-3.92425000	-1.43336600
C	8.02861300	-5.00088400	0.24914300
H	9.41722900	-0.04601200	1.87984400
C	10.65808500	1.20178100	0.65148400
H	11.32594400	-1.45734800	1.18169400
H	10.85718400	-1.29407700	-0.50779500
H	5.82142400	-4.75319700	-1.31119500
H	5.96919500	-3.03857600	-1.73753700
H	7.21073900	-4.19137300	-2.25200100
H	8.78909400	-5.27707000	-0.49285800
H	8.51494900	-4.95131200	1.22805400
H	7.29917600	-5.81836700	0.28626400
H	10.13619200	2.13389800	0.89810100
H	11.54009800	1.12911900	1.29895200
H	11.01093600	1.28108300	-0.38492200

1d'-c

B3LYP/6-31g(d),

el. energy = -2042.302473 a.u.

C	-0.69166300	2.36849900	-0.95140200
C	0.39934400	2.86841800	1.35153300
H	0.85688200	3.07921400	2.32197800
H	-1.15107900	2.15765700	-1.92018600
C	-1.52056800	1.84558700	0.22495100
C	-0.92712200	2.11554800	1.46913400
C	-2.72925000	1.17087000	0.12720400
C	-1.55967200	1.69952300	2.63273800
C	-3.36719600	0.75162800	1.31000700
H	-3.18655300	0.96476600	-0.83139500
C	-2.77730700	1.01891100	2.55297900
H	-1.11756100	1.89853300	3.60607400
H	-3.27322200	0.69318400	3.46502700
C	1.28566200	2.00930200	0.44686100
C	0.69401000	1.73797300	-0.79820300
C	2.54187800	1.51369300	0.75309400
C	1.37838200	0.96601800	-1.72643400
C	3.23441700	0.72936300	-0.19068600
H	2.99613600	1.72671100	1.71961800
C	2.64948500	0.45707200	-1.43348400
H	0.93193500	0.74772800	-2.69371100
H	3.18477000	-0.14563200	-2.15380800
C	-0.50177500	3.86561500	-0.69450900
C	0.09200500	4.13665400	0.55098100
C	-0.84880000	4.90681100	-1.54636600
C	0.33810900	5.44712600	0.94096400
C	-0.60071600	6.22912600	-1.15332100
H	-1.30890400	4.69788500	-2.50935000
C	-0.01157100	6.49757200	0.08139200
H	0.79728800	5.65679700	1.90447400
H	-0.86990200	7.04747300	-1.81585000
H	0.17816200	7.52493300	0.38084900
N	-4.59363300	0.05622000	1.31463200
H	-4.95848700	-0.20857900	2.21942100
N	4.50841100	0.25750400	0.18767300
H	4.82843800	0.51362700	1.11164200
C	-5.39151900	-0.28194800	0.25024600
C	5.36914800	-0.54419900	-0.51909400
O	5.19148500	-0.99764200	-1.63451400
O	-5.17921300	-0.04206700	-0.92417600
O	6.48137700	-0.75059000	0.24003500
C	7.49388000	-1.63439500	-0.31397400
C	8.88374100	-1.19579100	0.18712400
C	7.13525100	-3.07199700	0.07395900
H	7.45349200	-1.52922400	-1.40342400
C	9.90640800	-2.22740200	-0.34757300
H	8.88527400	-1.27487600	1.28600600
C	9.22185500	0.28464800	-0.19044700
C	8.16906900	-4.08927500	-0.43295400

H	7.06626700	-3.13150400	1.17008000
H	6.14194100	-3.30466200	-0.32727200
C	9.56695800	-3.67212200	0.04544900
H	10.90514900	-1.97927500	0.02449500
H	9.95766400	-2.15440600	-1.44444900
H	8.73490400	0.49470300	-1.15500100
C	8.67037200	1.28082300	0.84646600
C	10.72539500	0.55901700	-0.37613100
H	8.16611300	-4.05190600	-1.53393400
C	7.81137400	-5.51734600	-0.00682700
H	10.32494800	-4.35388100	-0.36268700
H	9.61545100	-3.77313400	1.14073700
H	8.86445000	2.31317500	0.53145000
H	7.59572100	1.16429600	0.99396900
H	9.16319200	1.13473100	1.81715000
H	11.28915900	0.34575300	0.54143100
H	11.16697900	-0.02769100	-1.18728300
H	10.88130100	1.61759600	-0.61452700
H	6.82024200	-5.80664800	-0.37556500
H	8.53857800	-6.24038300	-0.39520400
H	7.80069600	-5.60992600	1.08691700
O	-6.47805600	-0.94978700	0.72727000
C	-7.48530100	-1.34057500	-0.24574400
C	-8.14740400	-2.65712900	0.20539900
C	-8.47539600	-0.18141100	-0.39338900
H	-6.96889500	-1.50404000	-1.19754800
C	-9.28022900	-2.96596000	-0.80334300
H	-8.62162900	-2.47696900	1.18336100
C	-7.11781100	-3.82303200	0.37543200
C	-9.61411900	-0.50529400	-1.37278000
H	-8.89527600	0.04805700	0.59694400
H	-7.92588200	0.70700800	-0.72645000
C	-10.28844000	-1.81752000	-0.94836300
H	-9.80995100	-3.87161400	-0.49251600
H	-8.84079500	-3.18680200	-1.78783600
H	-6.32417500	-3.66890800	-0.37160300
C	-6.46501700	-3.81365000	1.77029200
C	-7.70634400	-5.22342800	0.12421900
H	-9.16797700	-0.66380800	-2.36747300
C	-10.61219400	0.65275400	-1.48052800
H	-11.06359600	-2.09591000	-1.67467700
H	-10.80389800	-1.66102600	0.01183400
H	-5.70577200	-4.60128900	1.84634000
H	-5.98936700	-2.85752500	1.99338800
H	-7.21798800	-4.00630500	2.54639100
H	-8.52865900	-5.44405100	0.81731000
H	-8.08190400	-5.34950400	-0.89570500
H	-6.93306300	-5.98355300	0.28522500
H	-10.11805700	1.57572500	-1.80609000
H	-11.40668700	0.42485800	-2.20111400
H	-11.08801000	0.85277600	-0.511754

3. NMR spectra of known and new compounds

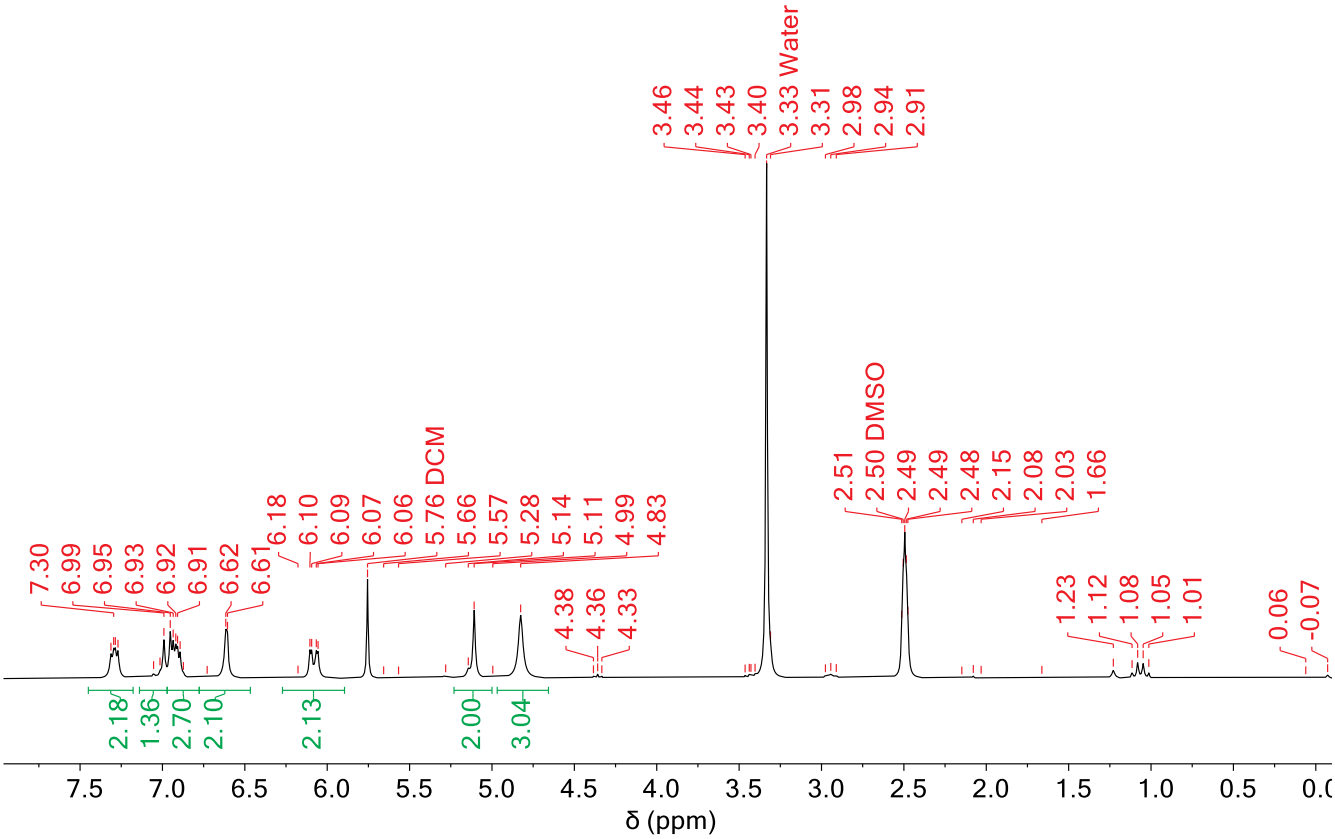

Figure S5. ^{1}H-NMR of compound **Tripty-NH2**.

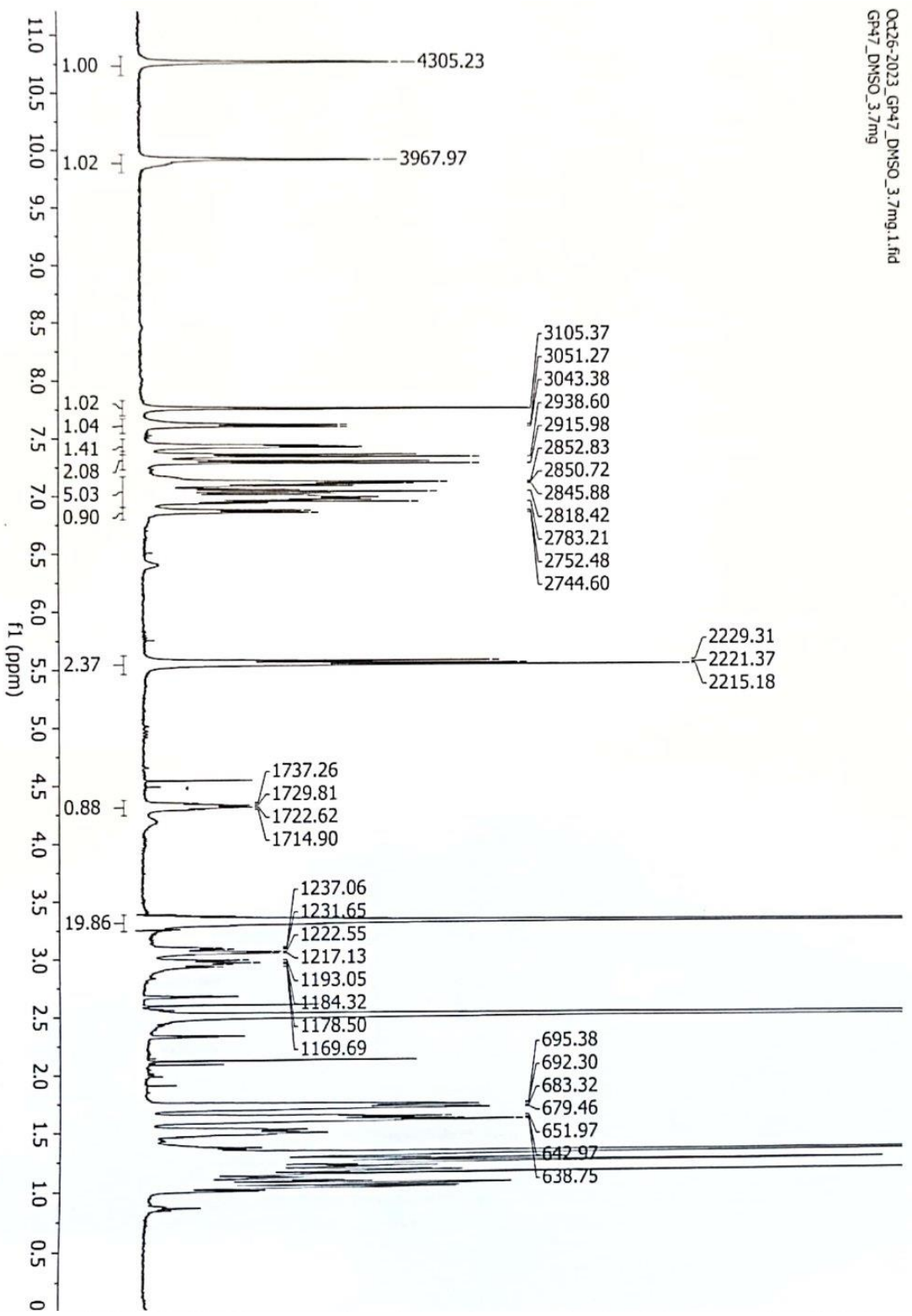

Figure S6. ^{1}H-NMR of compound **1a**.

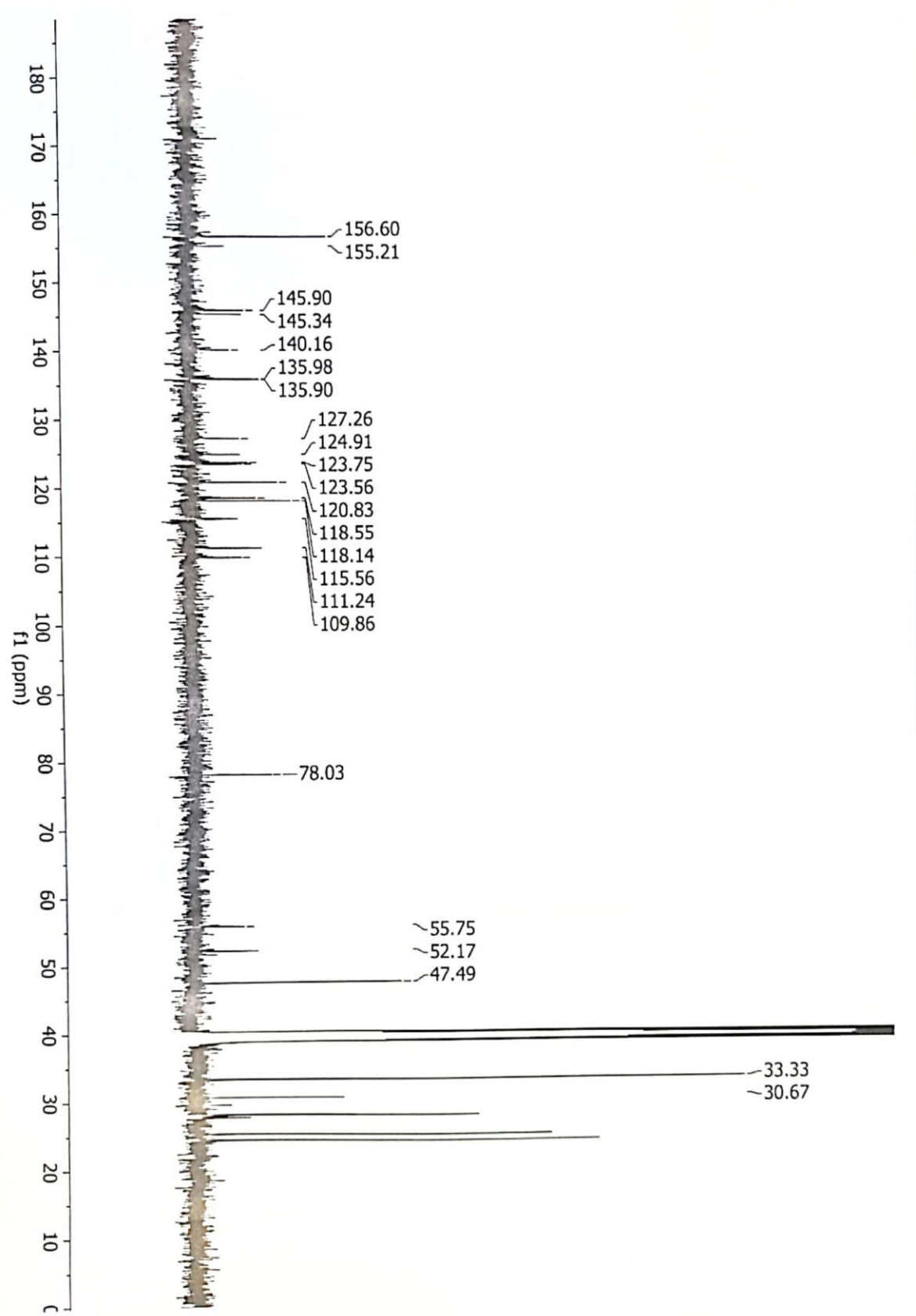

Figure S7. ^{13}C-NMR of compound **1a**.

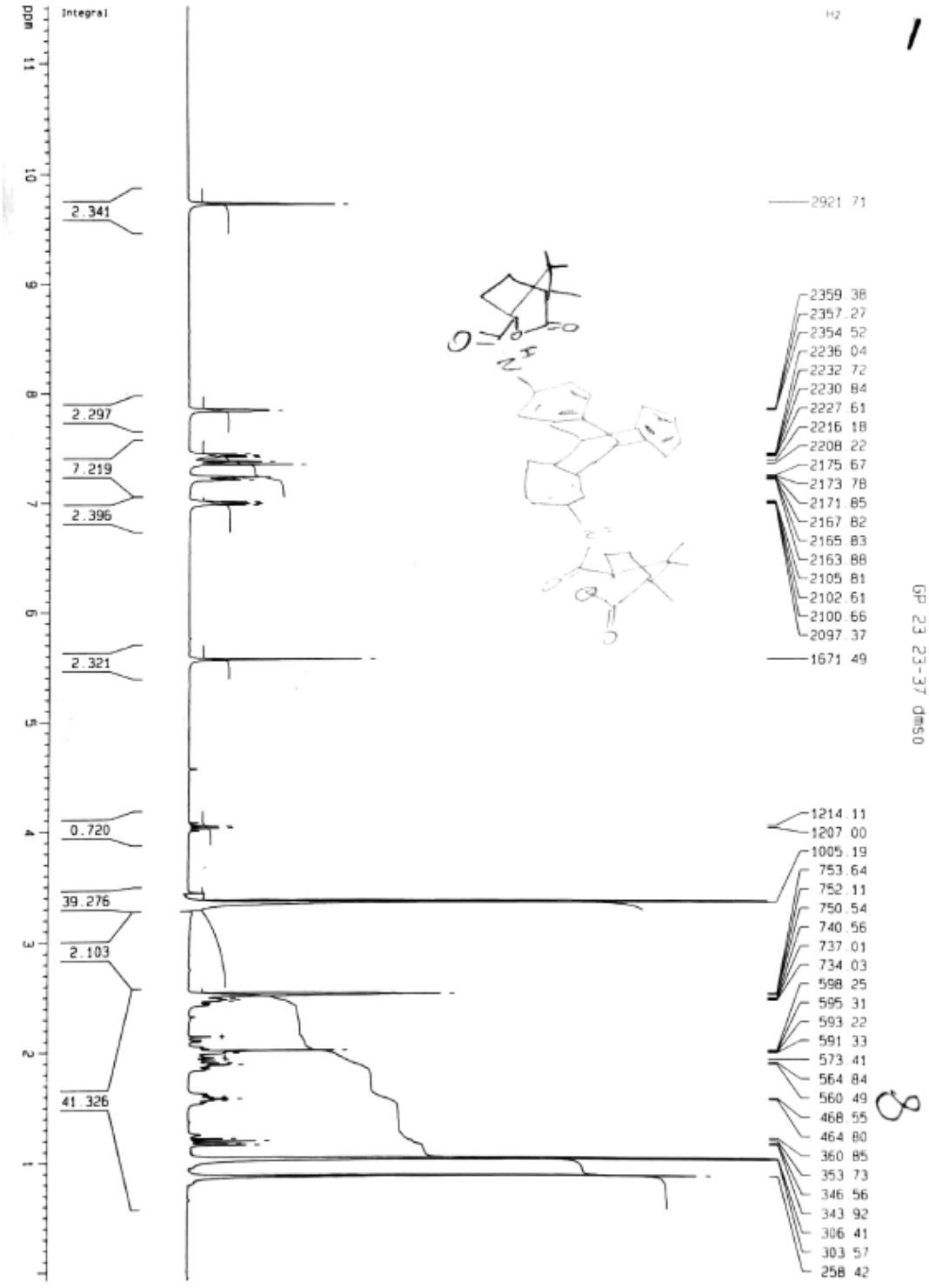

Figure S8. ^{1}H-NMR of compound **1b**.

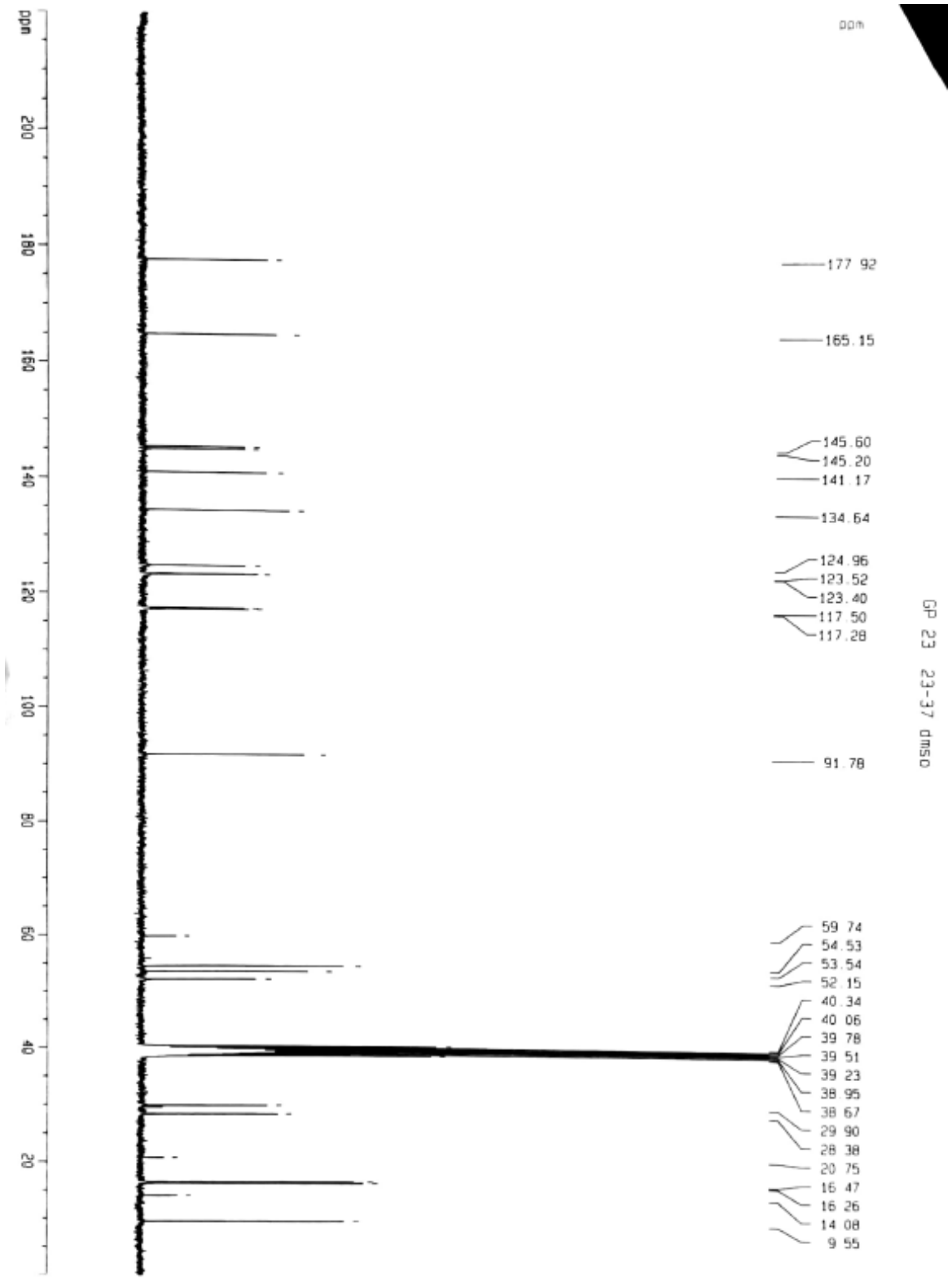

Figure S9. ^{13}C-NMR of compound **1b**.

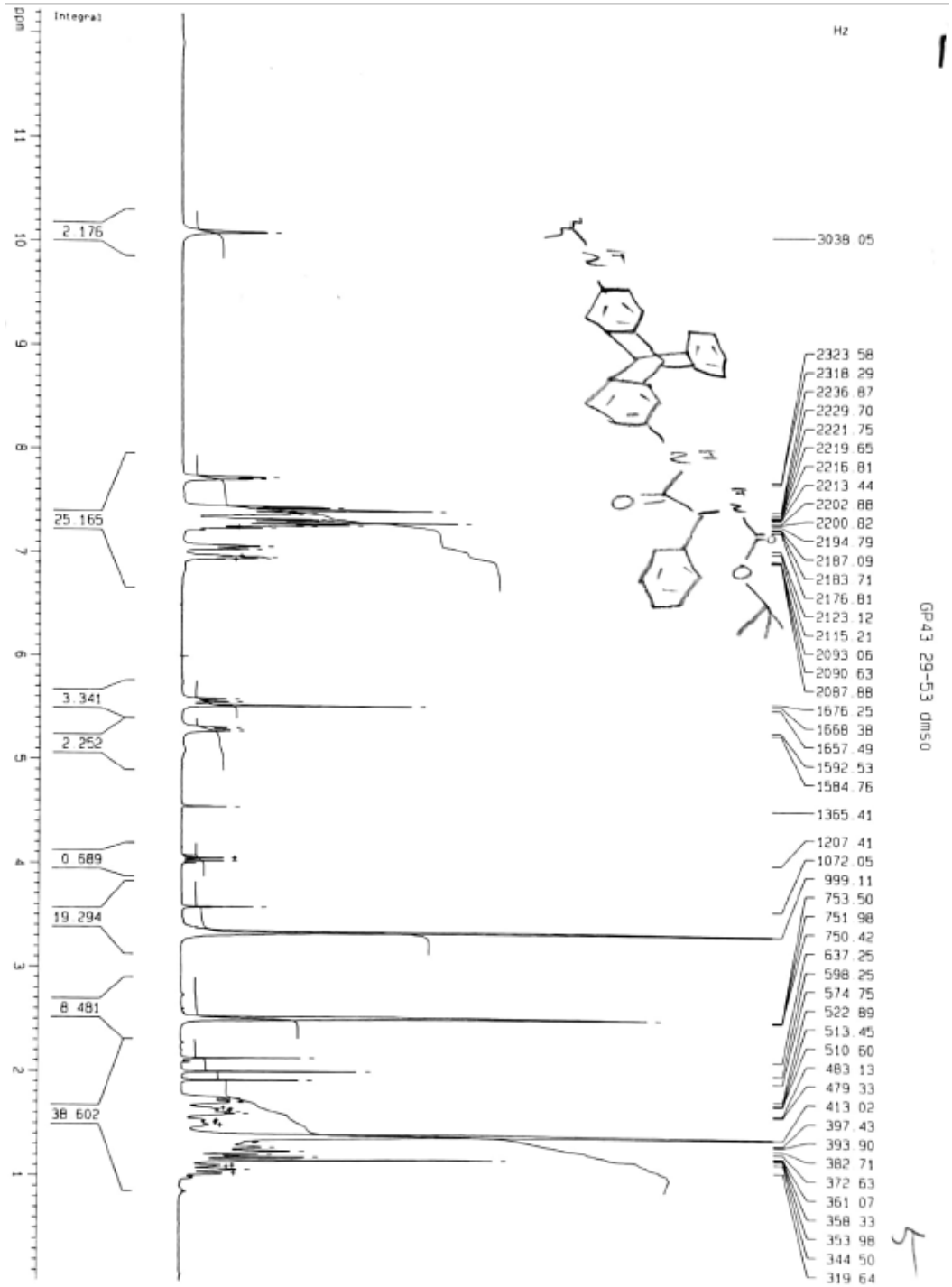

Figure S10. ^{1}H-NMR spectrum of **1c**.

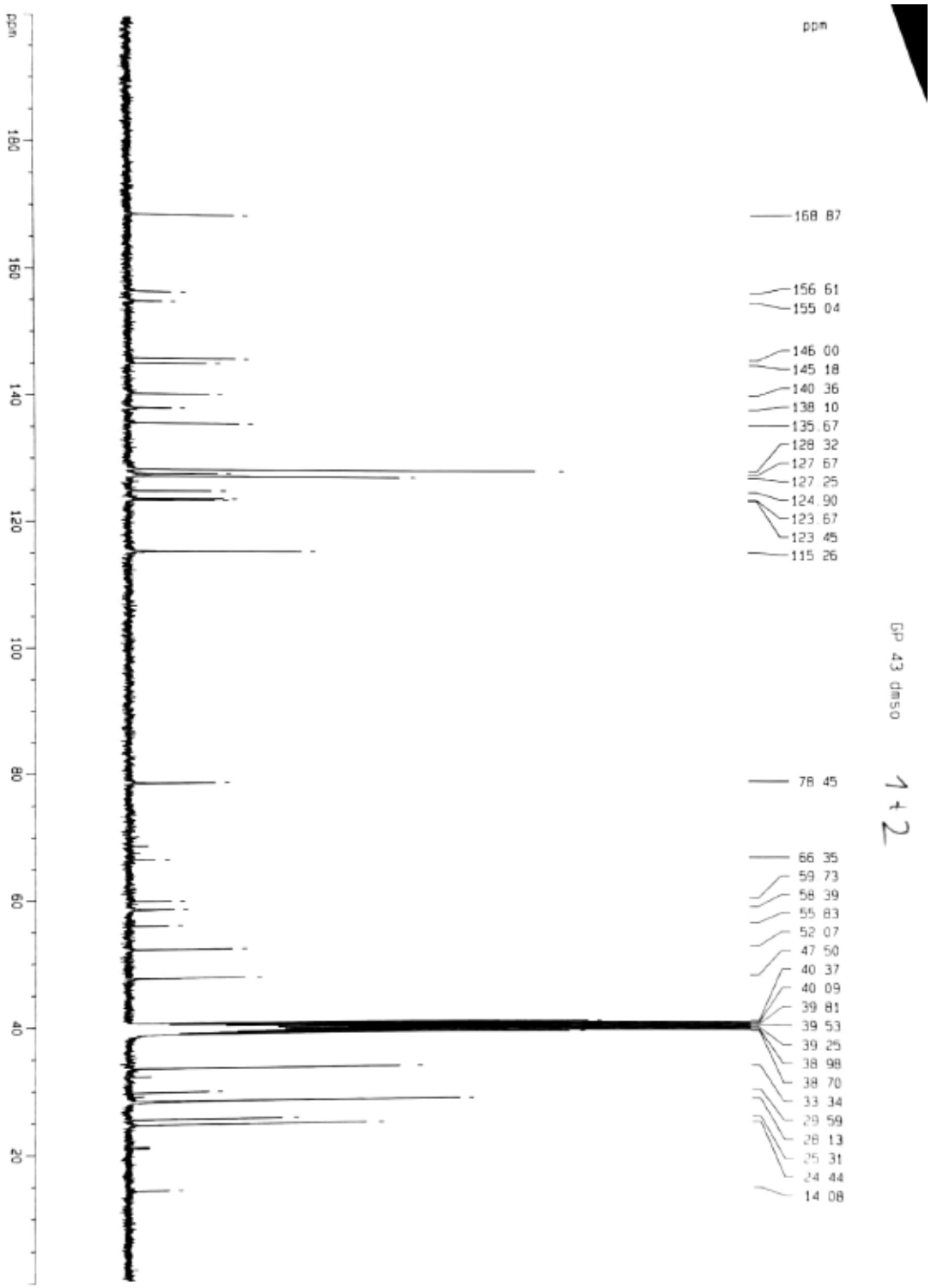

Figure S11. ^{13}C-NMR spectrum of **1c**.

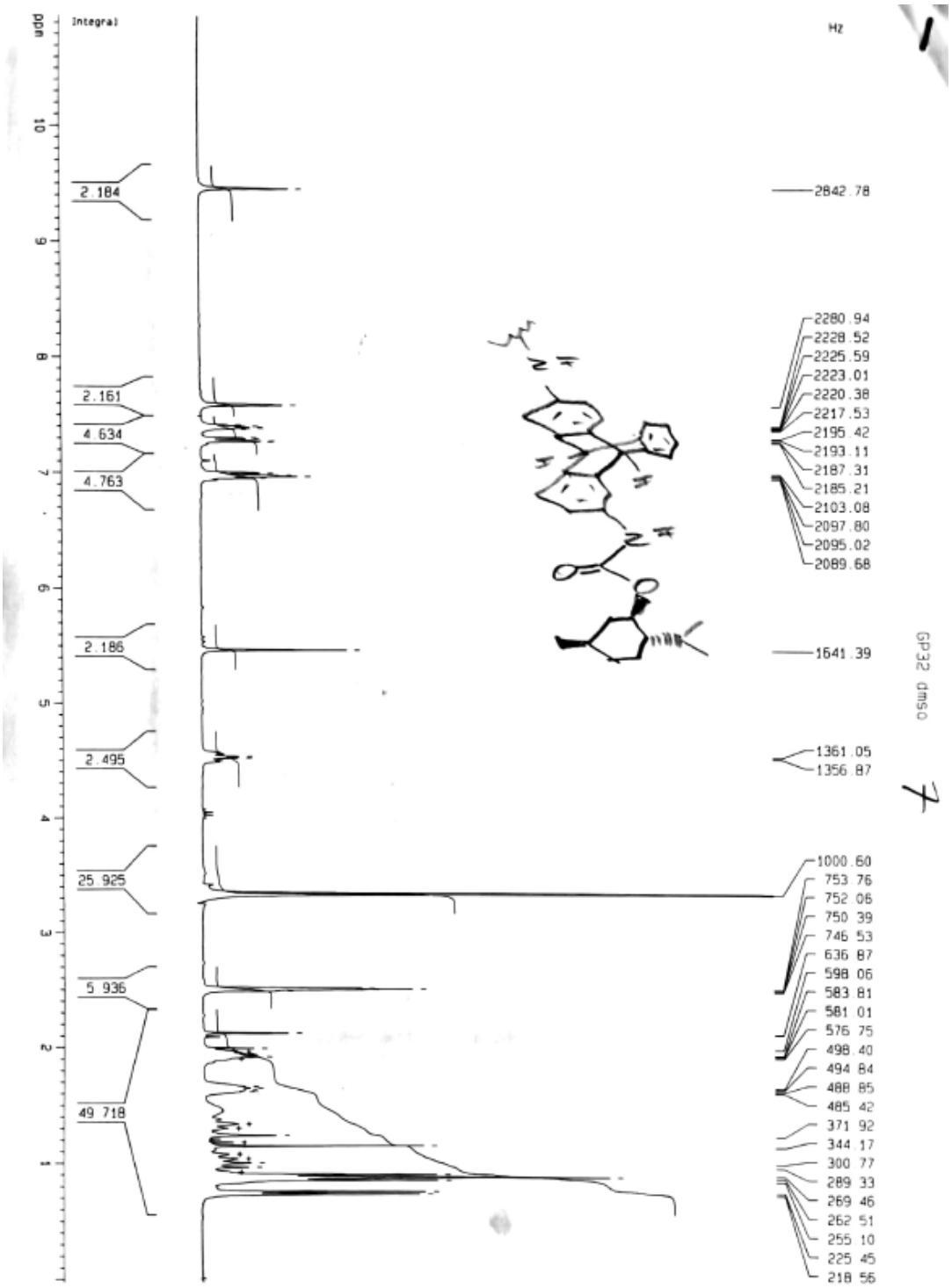

Figure S12. ^{1}H-NMR spectrum of **1d**.

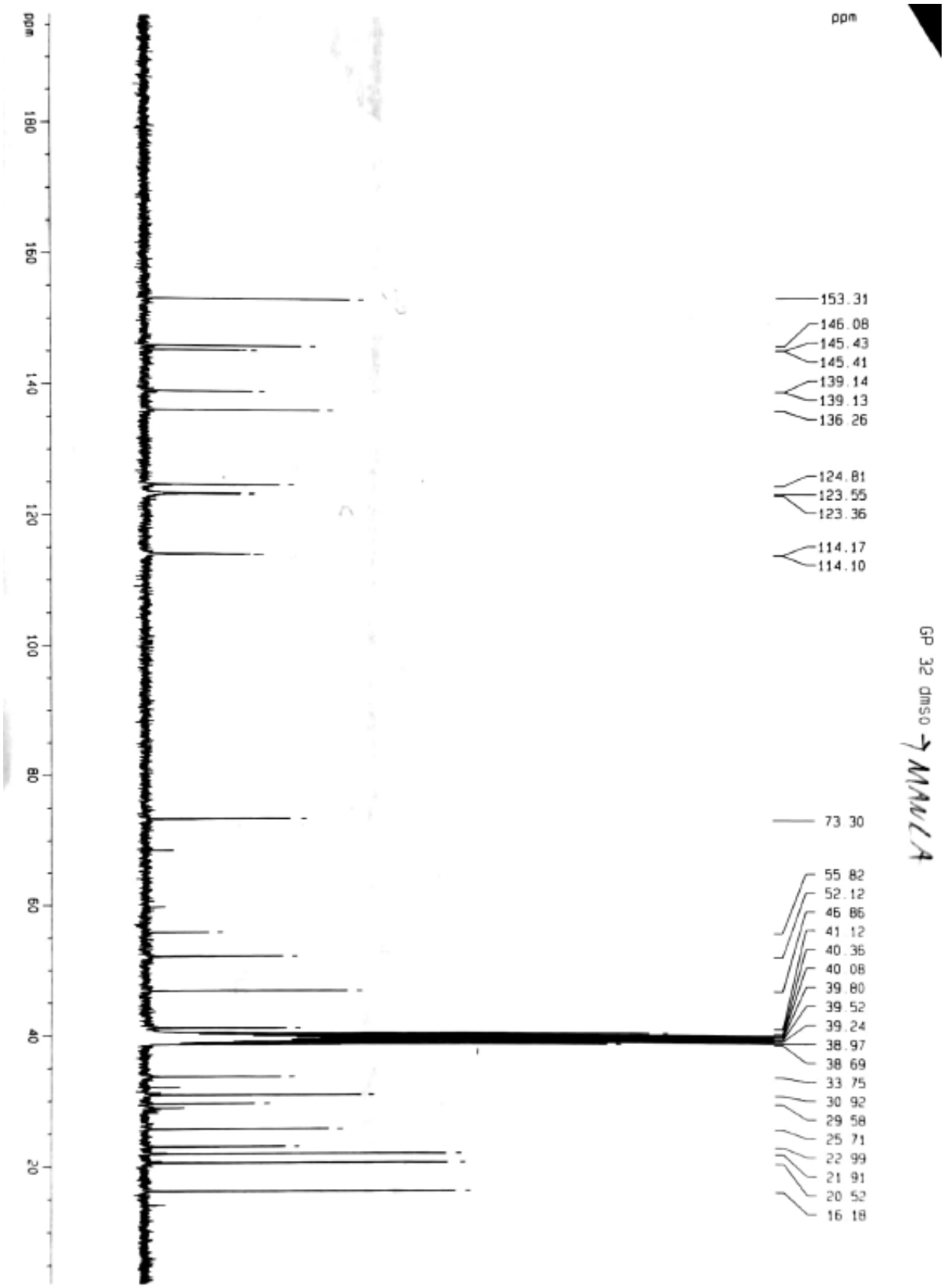

Figure S13. ^{13}C-NMR spectrum of **1d**.

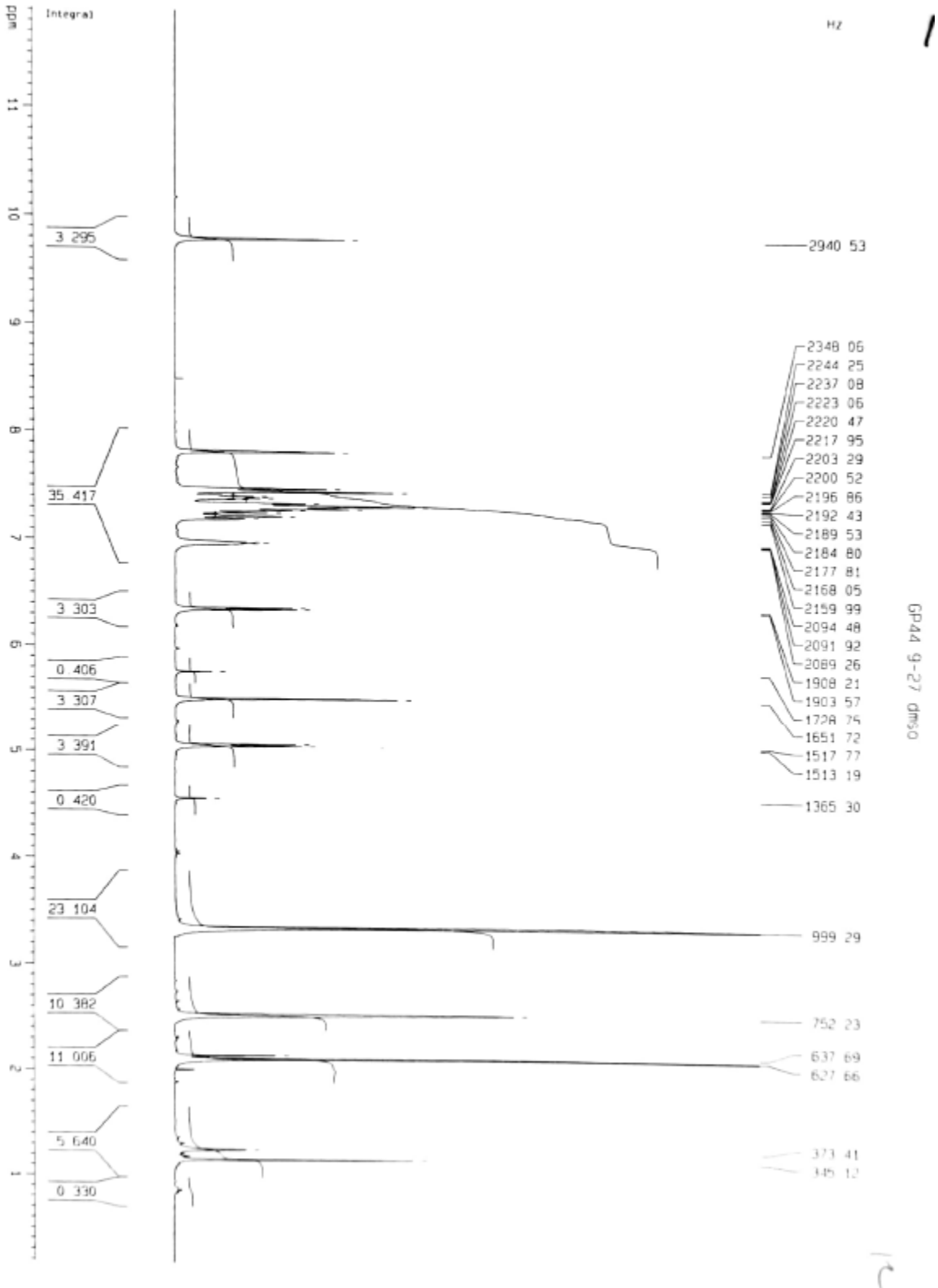

Figure S14. ^{1}H-NMR spectrum of **1e**.

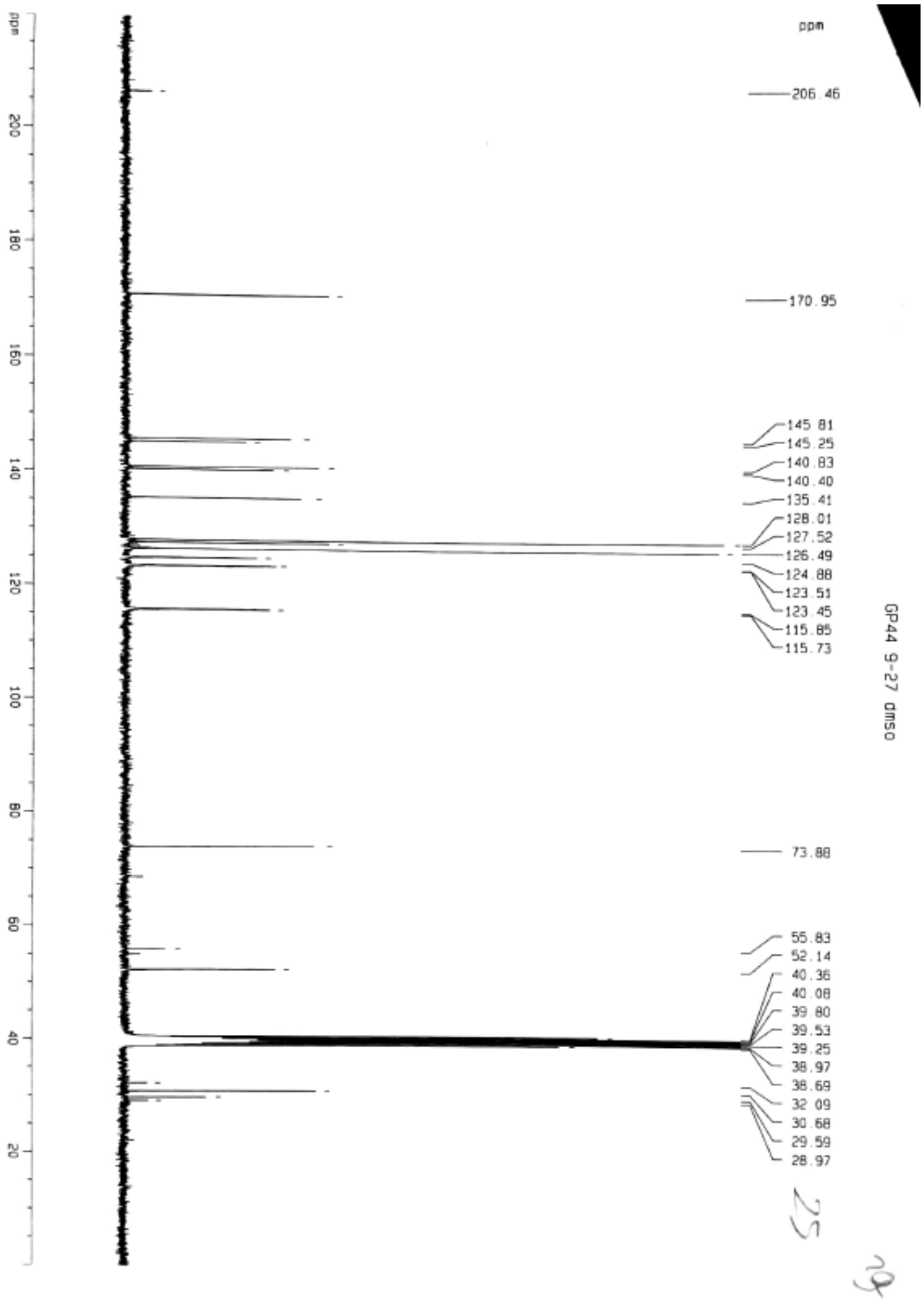

Figure S15. [1]HNMR spectrum of **1e**.

Mass spectra of new compounds

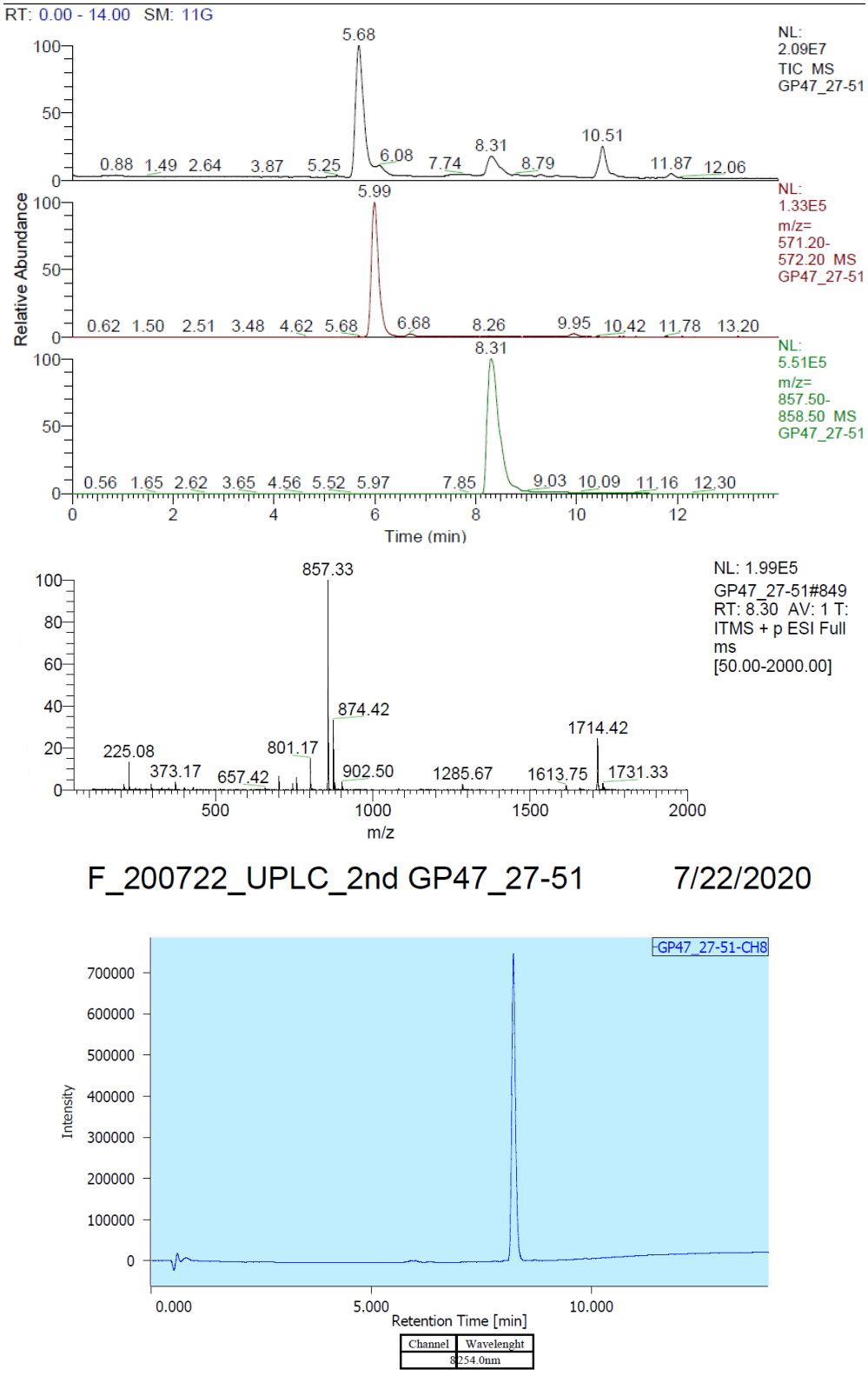

Figure S16. Mass spectrum and UPLC-UV-vis chromatogram of **1a**.

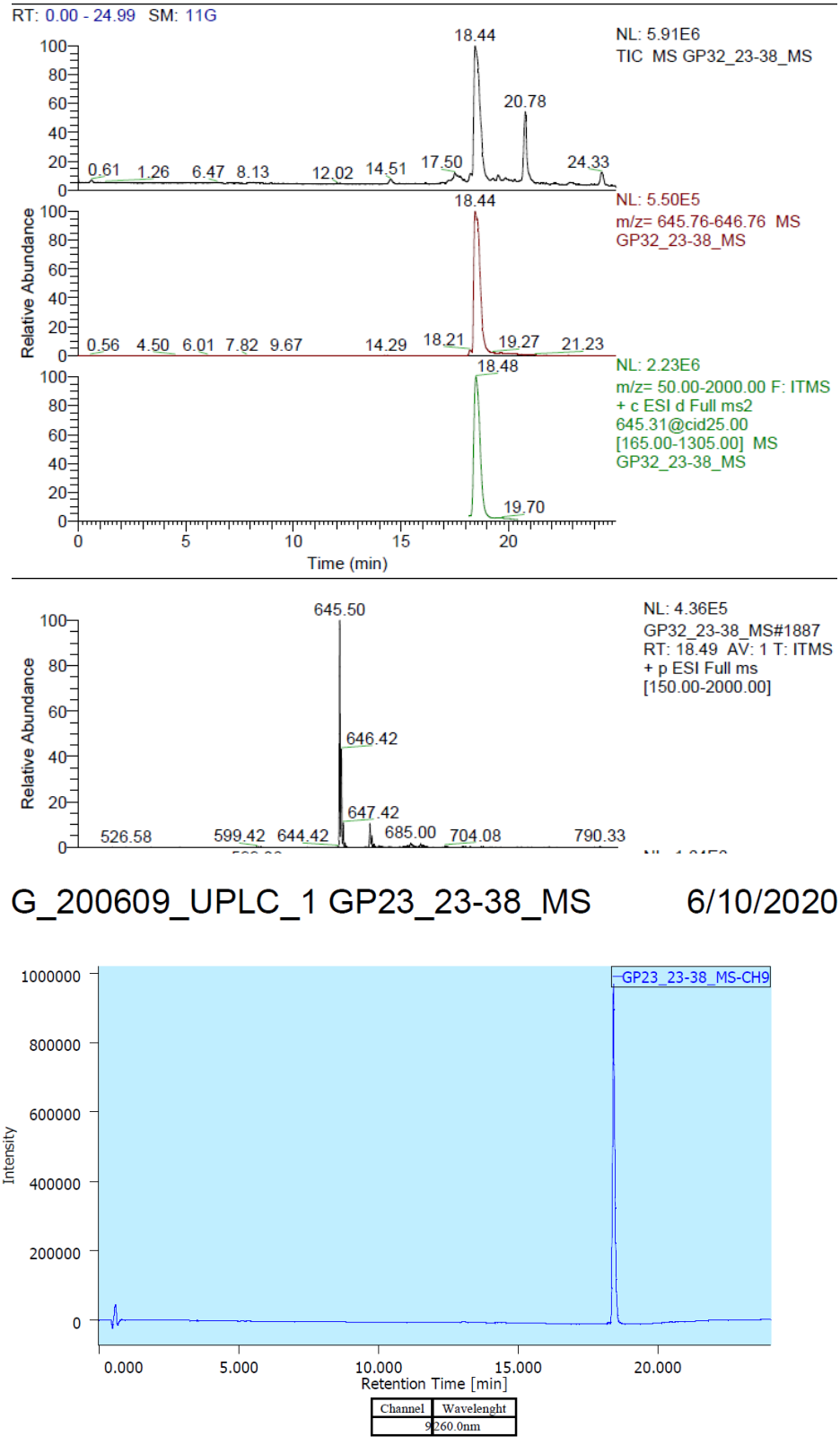

Figure S17. Mass spectrum and UPLC-UV-vis chromatogram of compound **1b**.

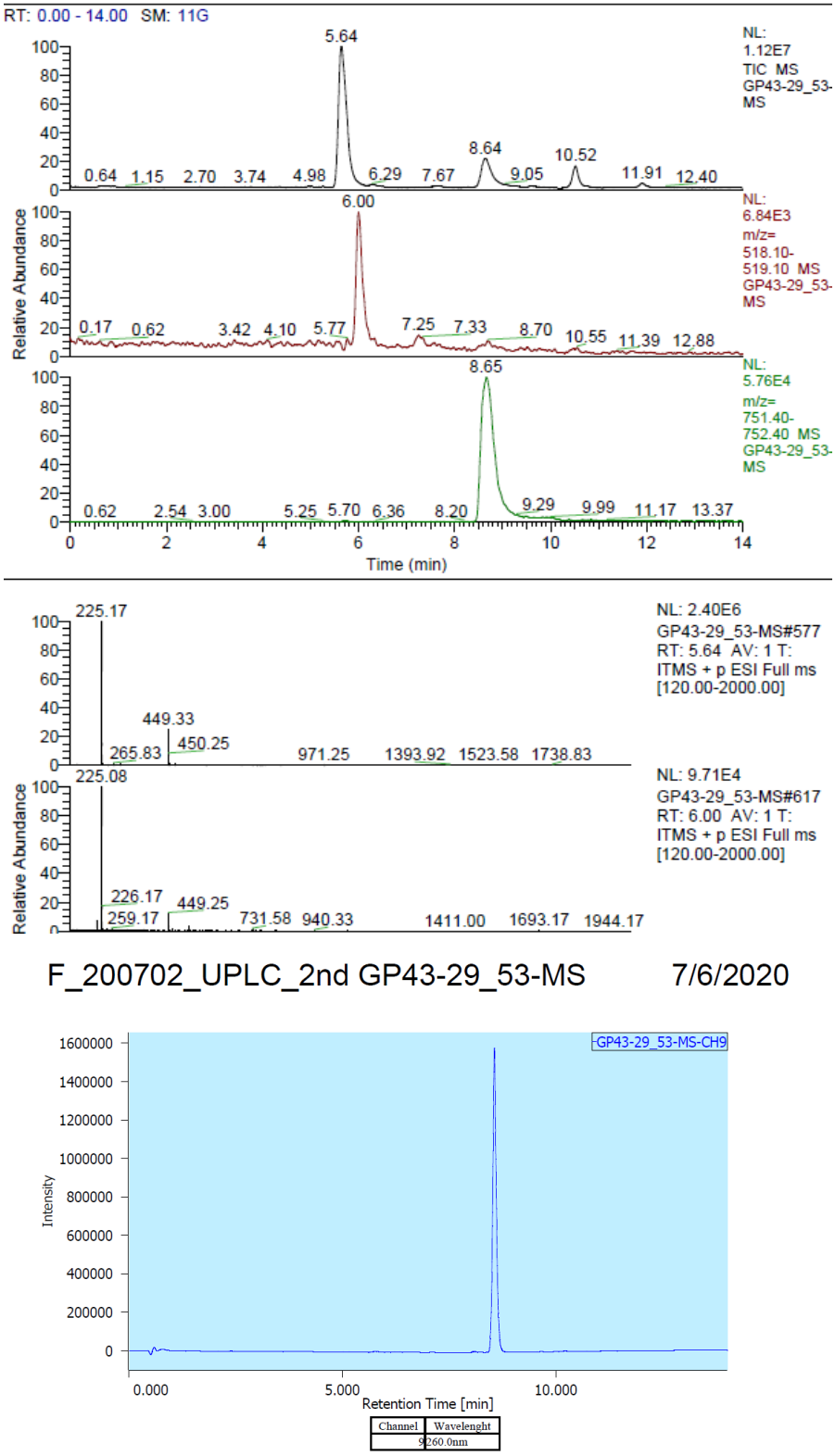

Figure S18. Mass spectrum and UPLC-UV-vis chromatogram of **1c**.

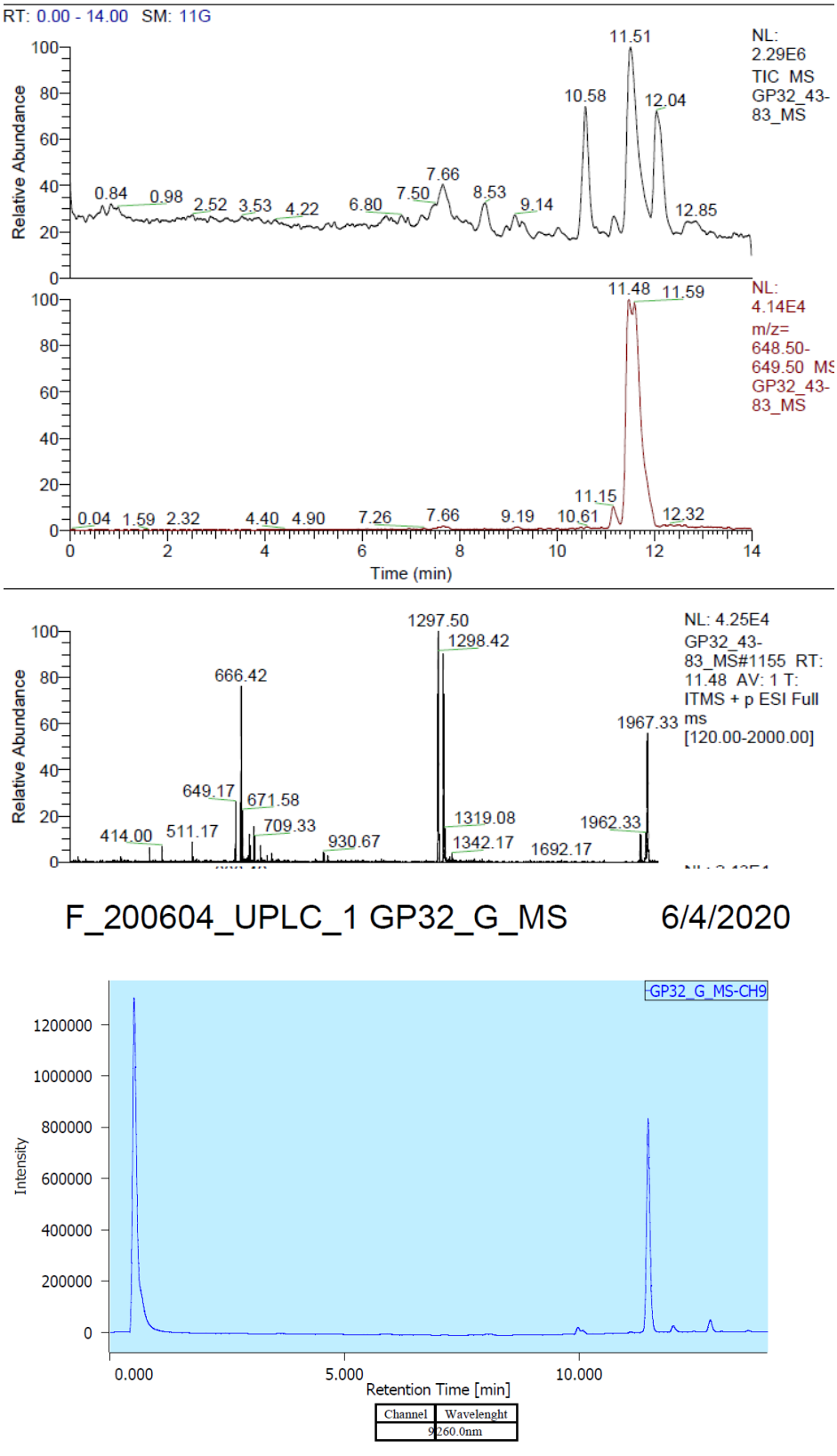

Figure S19. Mass spectrum and UPLC-UV-vis chromatogram of **1d**.

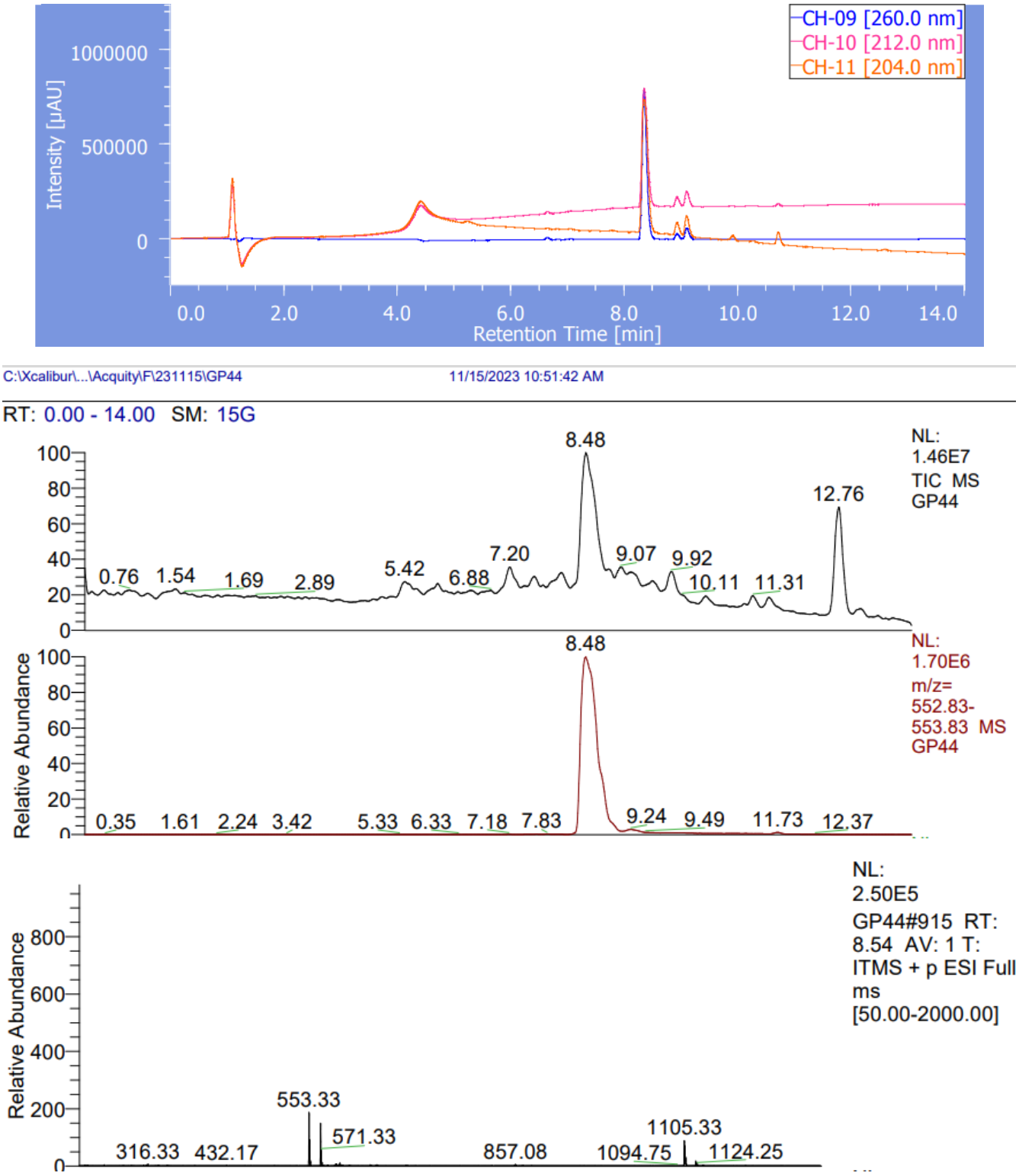

Figure S20. Mass spectrum and UPLC-UV-vis chromatogram of **1e**.