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Published in:
Analytica Chimica Acta

DOI:
10.1016/j.aca.2020.07.024

Published: 02/10/2020

Document Version
Accepted author manuscript

Document License
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Link to publication

Please cite the original version:
Tshepelevitsh, S., Kadam, S., Darnell, A., Bobacka, J., Rüütel, A., Haljasorg, T., & Leito, I. (2020). Log*P* determination for highly lipophilic hydrogen-bonding anion receptor molecules. *Analytica Chimica Acta*, *1132*, 123-133. https://doi.org/10.1016/j.aca.2020.07.024

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Supporting Information for

Log*P* Determination for Highly Lipophilic Hydrogen Bonding Anion Receptor Molecules

Sofja Tshepelevitsh, Sandip A. Kadam, Astrid Darnell, Johan Bobacka, Alo Rüütel, Tõiv Haljasorg, Ivo Leito

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Table S1. Computational and experimental details for all studied compounds

Notations: **BS** – basis set used for geometry optimization; **Conf.** – number of conformers taken into account; **logk_{80}** – directly measured or extrapolated retention factor at 80% MeOH in the eluent; ***S*** – slope of the log$k$ vs ϕ dependence; **ϕ range** – limits of ϕ values used in calculation of S and extrapolations; **N** – number of used data points.

Compound	CAS	Synthesis	Anion binding	COSMO-RS						Chromatography					Literature		Recommended log$P_{o/w}$[g]
				BS	Conf.	log$P_{o/w}$ [a]	Corrected log$P_{o/w}$[b]	log$P_{m/w}$ (CZ10&NPOE)[c]	log$P_{m/w}$ (CZ10&DOS)[c]	logk_{80}	$S\cdot10^3$	ϕ range	N	log$P_{o/w}$[d]	log$P_{o/w}$[e]	pK_{aH}[f]	
IC01	2099104-50-2	[1]	[1]	tzvp	6	9.9	8.8	9.1	8.6								8.8 (±2)
IC02	2098495-23-7	[1]	[1]	tzvp	6	10.4	9.2	9.6	9.2								9.2 (±2)
IC03	2098490-62-9	[1]	[1]	tzvp	6	11.4	10.1	10.7	10.3								10.1 (±2)
IC04	2098492-93-2	[1]	[1]	tzvp	2	10.3	9.1	9.4	9.0								9.1 (±2)
IC05	2099104-51-3	[1]	[1]	tzvp	10	8.8	7.8	6.5	5.3								7.8 (±2)
IC06	2098490-41-4	[1]	[1]	tzvp	9	9.8	8.7	7.8	6.9								8.7 (±2)
IC07	2098491-70-2	[1]	[1]	tzvp	2	8.5	7.6	7.6	7.2								7.6 (±2)
IC08	2098489-02-0	[1]	[1]	tzvp	2	7.3	6.5	6.0	5.5	0.63	-66	80-100	3	7.6			7.0 (±2)
IC09	60511-85-5	[2]	[2], [3], [4], [5]	tzvp	1	4.8	4.3	4.3	4.2	0.36	-47	70-90	4	5.1			4.7 (±1)
CZ01	1709799-61-0	[3]	[3], [4]	tzvp	8	8.9	7.9	8.0	7.8	1.14	-87	80-100	3	8.6			8.2 (±1)
CZ02	1709799-62-1	[3]	[3]	tzvp	5	15.9	14.0	16.1	15.8	2.22	-109	90-100	3	12.9			13.5 (±2)
CZ03	1709799-63-2	[3]	[3], [4]	tzvp	10	10.7	9.5	8.1	7.6	1.19	-86	80-100	4	9.9			9.7 (±1)
CZ04	2197988-18-2	[4]	[4]	tzvp	6	8.5	7.5	6.8	6.3	0.78	-75	80-100	3	8.1			7.8 (±1)
CZ05	(new compound)	this work		svp	4	8.9	7.9	7.6	7.0								7.9 (±2)
CZ06	(new compound)	this work		svp	7	10.4	9.2	10.3	9.9								9.2 (±2)
CZ07	(new compound)	this work		tzvp	5	8.6	7.6	8.1	7.4								7.6 (±1)
CZ08	1456532-80-1	[3]	[3], [4]	tzvp	7	14.5	12.8	13.5	13.1	2.11	-119	90-100	3	13.0			12.9 (±1)
CZ09	(new compound)	this work		svp	5	22.4	19.6	21.2	21.2	3.25	-141	95-99	6	16.0			18 (±3)
CZ10	2098494-22-3	[1]	[1], [4], [6]	tzvp	10	15.9	14.0	13.9	13.5	1.94	-115	85-95	4	13.9			13.9 (±1)
CZ11	2098490-63-0	[1]	[1], [4]	svp	10	14.0	12.3	12.3	11.7	1.77	-105	90-100	8	12.5			12.4 (±1)
CZ12	(new compound)	this work		svp	11	15.6	13.7	14.9	14.3								13.7 (±2)
CZ13	(new compound)	this work		svp	6	21.2	18.6	20.6	20.5	3.87	-171	95-100	3	18.3			18.5 (±2)
CZ14	(new compound)	this work		svp	3	27.9	24.4	27.3	27.6	4.90	-199	96-100	7	21.2			23 (±3)
CZ15	1154733-14-8	[3]	[3], [4], [7], [8], [9]	tzvp	6	6.0	5.4	5.4	5.1	0.17	-55	70-100	5	5.8			5.6 (±1)
CZ16	1456532-81-2	[1]	[1]	svp	4	10.2	9.0	9.2	8.7	1.52	-106	80-95	3	10.9			10.0 (±2)
MC01		[10], this work	[10]	svp	2	10.9	9.6	9.6	9.0	1.04	-80	80-100	4	9.2			9.4 (±1)
MC02		[10]	[10]	svp	3	20.9	18.4	17.9	17.6								18 (±3)
MC03		[10]	[10]	svp	6	12.3	10.9	11.2	11.0								10.9 (±2)
MC04		[10], this work	[10]	svp	6	12.4	10.9	10.7	10.4	1.80	-106	85-95	3	11.8			11.4 (±2)
MC05		[10]	[10]	svp	6	11.8	10.4	10.2	9.8								10.4 (±2)
MC06		[10]	[10]	svp	6	12.1	10.7	10.9	10.3								10.7 (±2)
MC07		[10]	[10]	svp	6	13.8	12.1	12.5	11.9								12.1 (±2)
MC08		[10]	[10]	svp	7	13.0	11.4	12.1	11.6								11.4 (±2)
MC09		[10]	[10]	svp	7	15.1	13.3	14.5	14.0								13.3 (±2)
MC10		[10]	[10]	svp	8	15.3	13.4	13.9	13.7								13.4 (±2)

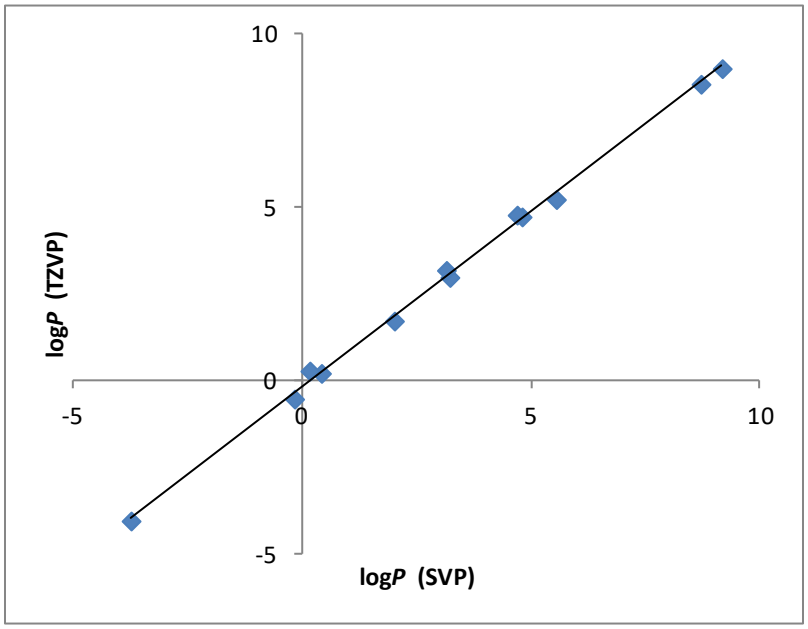
Compound	CAS	Synthesis	Anion binding	COSMO-RS						Chromatography					Literature		Recommended $\log P_{o/w}$[g]
				BS	Conf.	$\log P_{o/w}$ [a]	Corrected $\log P_{o/w}$[b]	$\log P_{m/w}$ (CZ10&NPOE)[c]	$\log P_{m/w}$ (CZ10&DOS)[c]	$\log k_{80}$	$S \cdot 10^3$	ϕ range	N	$\log P_{o/w}$[d]	$\log P_{o/w}$[e]	pK_{aH}[f]	
U01	1997362-24-9	this work		tzvp	6	4.5	4.1	4.5	4.0	-0.32	-42	60-100	6	3.7			3.9 (±1)
U02	1997362-25-0	this work		tzvp	5	1.7	1.6	0.1	-1.2	-1.19	-30	60-75	6	1.6			1.6 (±1)
U03	(new compound)	this work		tzvp	5	5.1	4.6	5.1	4.6	-0.25	-43	65-80	3	3.8			4.2 (±1)
U04	(new compound)	this work		tzvp	6	1.7	1.6	-0.2	-1.5								1.6 (±1)
U05	59239-63-3	this work		tzvp	5	2.8	2.6	1.3	0.6	-0.54	-35	65-80	3	2.7			2.7 (±1)
U06	64544-76-9	this work		tzvp	5	3.3	3.0	1.7	1.0	-0.57	-36	65-80	4	2.7			2.9 (±1)
U07	70980-65-3	this work		tzvp	3	4.0	3.7	2.7	2.0	-0.52	-39	60-100	9	3.0			3.3 (±1)
U10	91928-52-8	this work		tzvp	3	4.0	3.7	2.4	1.9	-0.21	-44	70-100	5	4.2			3.9 (±1)
U11	13140-79-9	this work	[11]	tzvp	4	3.8	3.5	1.9	1.2	-0.39	-42	65-80	4	3.9			3.7 (±1)
U12	614732-77-3	[4]	[4], [12], [13], [14], [15], [16]	tzvp	2	5.5	5.0	4.6	4.1	-0.42	-40	65-80	4	4.1			4.5 (±1)
U13	775322-64-0	[3]	[3], [4], [17], [18]	svp	3	7.2	6.5	7.5	7.0	0.07	-50	70-100	3	5.7			6.1 (±1)
U14	1827384-39-3	this work	[19]	tzvp	3	4.0	3.6	2.9	2.3	-0.33	-48	60-85	5	4.4			4.0 (±1)
U15	873797-28-5	[3]	[3], [20]	tzvp	6	5.7	5.1	5.9	5.4	-0.26	-43	70-90	4	4.5			4.8 (±1)
U16	948047-74-3	[3]	[3]	tzvp	7	2.2	2.1	0.8	-0.5								2.1 (±1)
U17	1709799-59-6	[3]	[3]	tzvp	4	4.8	4.3	3.5	3.0	-0.30	-44	60-100	6	4.2			4.3 (±1)
U18	13140-78-8	[21]	[3], [11], [21], [22], [23], [24]	tzvp	2	4.1	3.7	2.7	2.2	-0.43	-40	65-80	4	3.8			3.8 (±1)
U19	1044762-46-0	[3]	[3], [4], [8], [25]	tzvp	5	2.9	2.6	2.2	1.9	-0.46	-40	60-80	4	3.5			3.1 (±1)
U20	1709799-60-9	[3]	[3], [26]	tzvp	8	5.6	5.0	3.9	3.2	-0.10	-50	70-90	4	5.4			5.2 (±1)
U21	(new compound)	this work		tzvp	7	5.4	4.8	2.4	1.1	-0.44	-54	60-80	3	4.9			4.9 (±1)
U22	(new compound)	this work		svp	6	6.8	6.0	4.0	2.9	-0.36	-52	70-85	4	4.9			5.5 (±2)
U23	(new compound)	this work		tzvp	5	7.3	6.5	5.6	4.4	-0.29	-53	70-95	6	6.0			6.2 (±1)
U24	948047-75-4	[3]	[3], [4], [27]	svp	9	8.4	7.5	7.7	6.8	-0.39	-49	70-90	3	5.5			6.5 (±2)
U25	1709799-52-9	[3]	[3], [4]	tzvp	7	8.8	7.8	7.6	6.9	-0.11	-55	70-90	3	6.0			6.9 (±2)
U26	1709799-53-0	[3]	[3], [4]	svp	7	15.3	13.5	14.2	14.0	1.81	-95	85-100	4	10.6			12.0 (±2)
U27	2098492-98-7	[1]	[1]	tzvp	11	6.0	5.4	2.8	1.5	-0.26	-57	70-90	4	6.0			5.7 (±1)
U28	2099104-52-4	[1]	[1]	tzvp	7	6.5	5.8	3.7	2.7	-0.24	-54	70-100	4	5.9			5.9 (±1)
U29	1709799-54-1	[3]	[3]	tzvp	10	4.7	4.3	3.4	3.0	-0.35	-44	70-80	4	3.8		5.4	4.0 (±1)
U31	607-56-7	[3]	[3]	tzvp	6	5.0	4.5	3.5	3.1	-0.06	-44	70-90	4	4.5			4.5 (±1)
U32	78751-44-7		[28]	svp	3	8.0	7.1	6.6	6.2								7.1 (±1)
HZ01	170112-64-8	this work		tzvp	6	4.6	4.2	3.9	3.3	-0.42	-43	65-80	10	4.1			4.1 (±1)
HZ02	2937-77-1	this work		tzvp	2	2.5	2.3	1.7	0.9	-0.77	-31	65-80	3	2.4			2.3 (±1)
HZ03	2209-59-8	this work		tzvp	2	3.5	3.2	3.9	3.1	-0.34	-40	65-95	3	3.7			3.4 (±1)
HZ04	621-12-5	As in.ref. [29]		tzvp	3	3.2	3.0	2.8	2.3	-0.54	-39	60-90	4	2.9			2.9 (±1)
HZ05	79984-71-7	this work		tzvp	6	2.8	2.6	2.5	1.9	-0.61	-37	70-80	3	2.9			2.45 [h]
o-NPOE	37682-29-4		(plasticizer)	tzvp	1	5.3	4.8	5.9	5.6						5.9 ± 2 [30]		4.8 (±1)
DOS	122-62-3		(plasticizer)	tzvp	5	10.8	9.5	10.8	10.9						10.1 ± 2 [30]		9.5 (±1)
1-Aminopyrene	1606-67-3			tzvp	1	4.0				0.01	-38	70-80	3		4.31	4.3	
1-Naphthylamine	134-32-7			tzvp	1	2.5				-0.53	-30	60-80	6		2.25	3.92 [31]	
2'-Aminoacetophenone	551-93-9			tzvp	2	1.9				-0.68	-23	70-80	3		1.63	2.3	
2-Aminobenzophenone	2835-77-0			tzvp	2	3.4				-0.26	-34	70-90	3			0.3	2.99 [h]
4-Aminobiphenyl	92-67-1			tzvp	1	3.3				-0.35	-35	60-80	5		2.86	4.3	
4-CF_3-7-coumarinyl-N=P(Ph)$_2$pyrr	2417391-06-9	[32]		tzvp	4	6.9				0.50	-59	70-90	6		6.2 [32]	7.5 [32]	

Compound	CAS	Synthesis	Anion binding	COSMO-RS						Chromatography					Literature		Recommended $\log P_{o/w}$ [g]
				BS	Conf.	$\log P_{o/w}$ [a]	Corrected $\log P_{o/w}$ [b]	$\log P_{m/w}$ (CZ10&NPOE) [c]	$\log P_{m/w}$ (CZ10&DOS) [c]	$\log k_{80}$	$S \cdot 10^3$	ϕ range	N	$\log P_{o/w}$ [d]	$\log P_{o/w}$ [e]	pK_{aH} [f]	
4-CF_3-7-coumarinyl-N=P(Ph)$_3$	2417391-05-8	[32]		tzvp	2	7.4				0.45	-60	70-90	3		6.5 [32]	6.8 [32]	
Acetanilide	103-84-4			tzvp	2	1.6				-0.82	-22	50-90	7			0.5	1.19 [h]
Anthraquinone	84-65-1			tzvp	1	2.8				0.11	-31	70-90	3		3.3 [33]		
Carbazole	86-74-8			tzvp	1	3.8				-0.07	-37	60-100	4				3.52 [h]
Dihexyl phthalate	84-75-3			tzvp	3	7.0				0.96	-67	80-100	3		5.8		
Dimethyl phthalate	131-11-3			tzvp	3	1.7				-0.67	-27	60-80	3		1.56		
Dioctyl phthalate	117-84-0			tzvp	3	9.2				1.48	-81	80-100	3		8.06		
Diphenylamine	122-39-4			tzvp	1	4.1				-0.03	-39	60-80	3		3.50	0.79 [34]	
Etofenprox	80844-07-1			tzvp	5	8.3				1.05	-68	80-100	3		7.05		
Indole	120-72-9			tzvp	1	2.4				-0.49	-28	50-90	7			-2.4	2.21 [h]
N,*N*-Diphenylurea	102-07-8			tzvp	3	3.2				-0.44	-33	65-80	5				2.98 [h]
NO_2-Ph-N=N-Ph-N=P(Ph)$_3$	33341-94-5	[35]		tzvp	2	8.1				0.78	-66	80-95	3		7.8 [35]	7.3 [35]	
Phenytoin	57-41-0			tzvp	1	2.3				-0.70	-36	60-80	7			-2.8	2.42 [h]
Ph-N=N-Ph-N=P(Ph)$_3$	33341-95-6	[35]		tzvp	2	8.0				0.63	-61	80-95	3		7.2 [35]	7.7 [35]	
Trifluralin	1582-09-8			tzvp	5	5.4				0.63	-59	70-90	5		5.34	-1.5	
Triphenylamine	603-34-9			tzvp	1	6.2				0.75	-55	80-100	4		5.74	-3.0	
Triphenylphosphate	115-86-6			tzvp	2	5.7				0.05	-49	70-90	6		4.59		
U08	849-97-8	this work		tzvp	6	2.4		0.9	0.1	-0.61	-33	70-90	4				2.60 [h]
U09	24775-54-0	this work	[36]	tzvp	2	3.0		2.5	1.8	-0.75	-36	60-80	5				2.27 [h]
U30	1709799-55-2	[3]	[3]	svp	8	3.4		2.0	1.4	-0.60	-36	65-90	3				3.10 [h]
U33	1467-21-6	[3]	[3], [37]	tzvp	4	3.3		2.6	2.2	-0.50	-32	70-90	3				2.83 [h]

[a] Value obtained directly from COSMOtherm, without corrections.
[b] Calculated by COSMO-RS method, corrected using equation 2 (see the main text).
[c] Calculated by COSMO-RS. Membrane composition: ionophore (**CZ10**) 2% by mass, tridodecylmethylammonium chloride 50 mol% vs. ionophore, mass ratio of PVC to plasticizer – bis(2-ethylhexyl) sebacate (DOS) or 2-nitrophenyl octyl ether (o-NPOE) – 1:2, degree of polymerization of PVC - 900.
[d] Average of predictions by equations 3, 4 and 5 (see the main text).
[e] Values from ref. [38] if not stated otherwise.
[f] Values calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2017 ACD/Labs), if not stated otherwise.
[g] Average of the chromatographic and corrected COSMO-RS values, if not stated otherwise. Combined uncertainties at ca 90% coverage level were estimated depending on the absolute value (extent of extrapolation), agreement between the two methods and complexity of the compound structure (abundance of possible conformations, possibilities for intramolecular hydrogen bond formation).
[h] Value from this work, determined as described in ref. [33]; combined uncertainty at ca 90% level of confidence is ±0.08 log units.

Comparison of the results by TZVP and SVP basis sets

Comparison of the two basis sets in the context of log*P* calculation was carried out on the example of 4 molecules: **CZ07**, **U29**, **U02** and **U17**. The same set of starting geometries was optimized using TZVP and SVP basis sets, followed by the single-point calculation (BP86/def2-TZVPD-Fine). The obtained files were used for log*P* calculations in 3 binary systems: octanol/water, hexane/water and toluene/water at 25°C.



The correlation between the two obtained sets of log*P* values is as follows (standard errors in parenthesis):

log*P*(TZVP) = 1.01(0.01) · log*P*(SVP) – 0.18(0.07), R^2 = 0.9982, N = 12

The maximum absolute difference was 0.4 log units. It was thus concluded that using TZVP and SVP basis sets for geometry optimization gives insignificantly different results in the context of this work.

Table S2. Additional descriptors for retention-based models

From the pool of over 1800 descriptors obtainable with PaDEL, most were rejected for one of the following reasons:

- Constant value for all studied receptor molecules
- Physical meaning not obvious, difficult interpretation
- Strong correlation with some other descriptor
- 3D (value depends on the chosen conformation)

The following descriptors were considered for retention-based models:

Name	**Description** [a]
Mv	Mean atomic van der Waals volumes (scaled on carbon atom)
Mpe	Mean atomic Pauling electronegativities (scaled on carbon atom)
Mp	Mean atomic polarizabilities (scaled on carbon atom)
Mi	Mean first ionization potentials (scaled on carbon atom)
ETA_dBetaP	A measure of relative unsaturation content relative to molecular size
ETA_BetaP_ns_d	A measure of lone electrons entering into resonance relative to molecular size
ETA_dEpsilon_D	A measure of contribution of hydrogen bond donor atoms
ETA_Psi_1	A measure of hydrogen bonding propensity of the molecules and/or polar surface area
McGowan_Volume	McGowan characteristic volume
HybRatio	Fraction of sp3 carbons to sp2 carbons
nAtomP	Number of atoms in the largest pi system
nAtomLAC	Number of atoms in the longest aliphatic chain
nHBAcc	Number of hydrogen bond acceptors (using CDK HBondAcceptorCountDescriptor algorithm)
nHBDon	Number of hydrogen bond donors (using CDK HBondDonorCountDescriptor algorithm)
MLFER_A	Overall or summation solute hydrogen bond acidity
MLFER_BH	Overall or summation solute hydrogen bond basicity
MLFER_S	Combined dipolarity/polarizability
MLFER_E	Excessive molar refraction
TopoPSA	Topological polar surface area

[a] **http://www.yapcwsoft.com/dd/padeldescriptor/Descriptors.xls**

Correlations between calculated log$P_{m/w}$ and log$P_{o/w}$ values

Dashed black lines are *y* = *x* lines; solid blue lines are regression lines. Log$P_{o/w}$ values are calculated by COSMO-RS and corrected using Eq. 2 (see the main text).

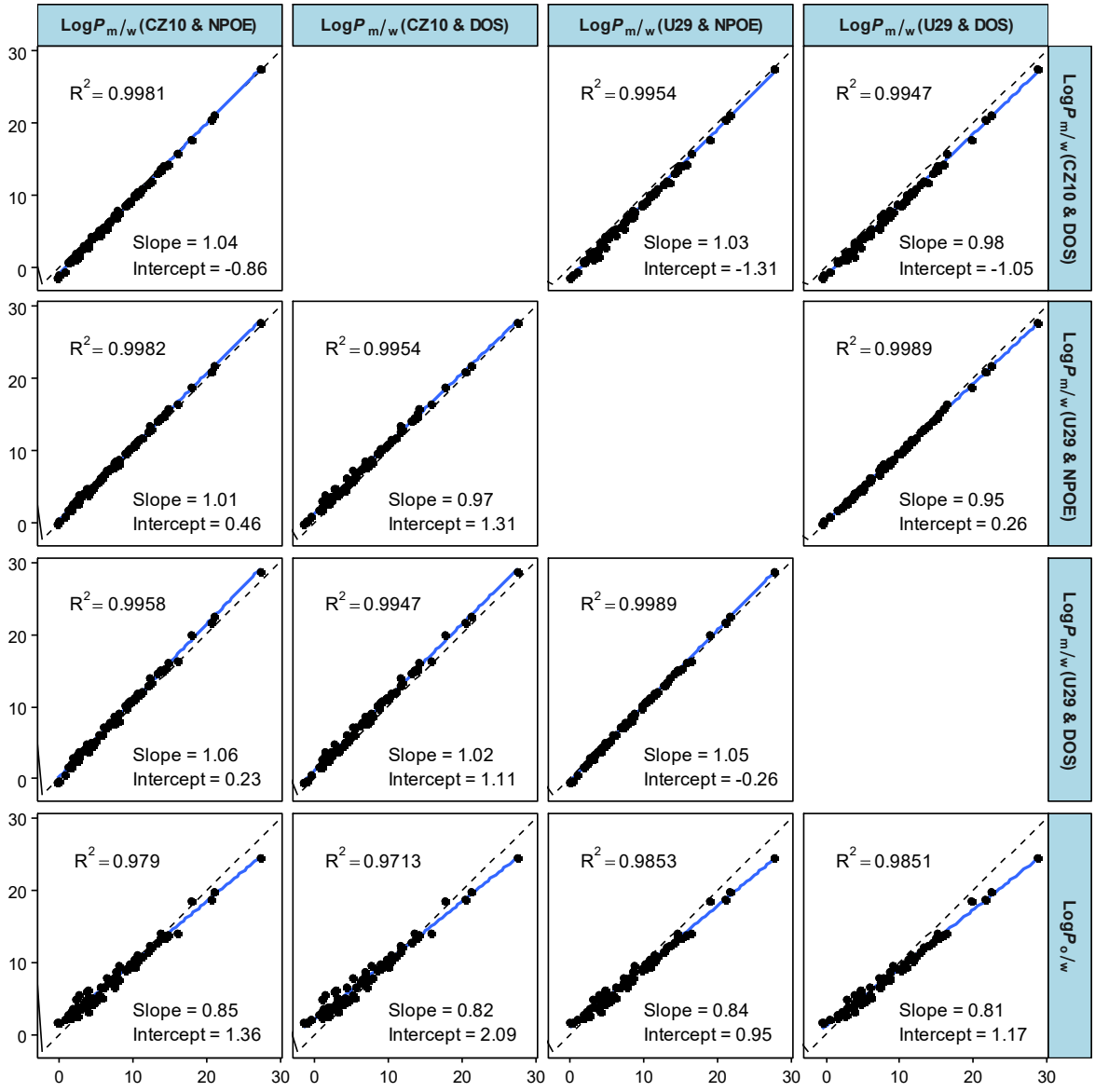
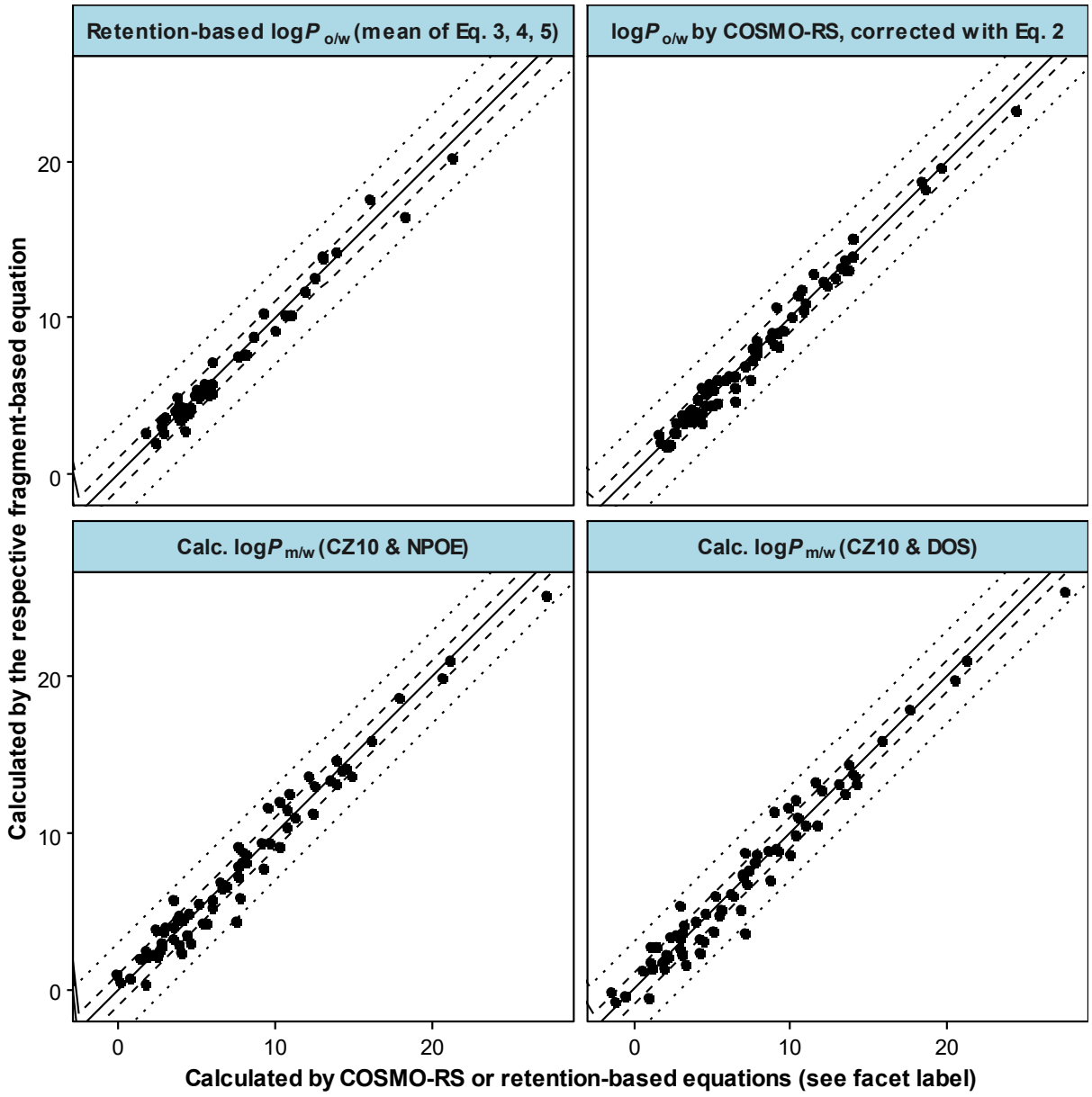


Table S3. All descriptors considered for „simple“ models

Name	Description
nC, nH, nO, nN, nS	Numbers of C, H, O, N, S atoms, respectively
Rings	Number of aromatic rings
Pyrr	Number of pyrrole rings (incl. in carbazole, indole, indolocarbazole moieties)
tBu	Number of tert-butyl groups
C	Number of C, CH, CH_2 and CH_3 that are NOT part of tert-butyl groups, carbonyl groups or aromatic rings
Urea	Number of ureylene (–NH-CO-NH–) and thio-ureylene (–NH-CS-NH–) fragments
CO-NH	Number of –CO-NH– fragments that are NOT part of ureylene fragments
CO	Total number of carbonyl (>C=O) groups
allNH	Total number of NH groups; amino group counts for 2
NH-NH	Number of NH groups in ortho position relative to each other; each NH with a "neighbour" counts; -NH_2 group counts for 2.
NO2	Number of nitro groups
NO2-NH	Number of nitro groups in ortho position to NH group
MW	Molar mass

Performance plots for the „simple“ models

Solid lines are *y* = *x* lines; dashed lines mark the 1-unit distance and dotted lines 3-unit distance from the *y* = *x* lines.



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Synthesis and characterization data

Abbreviations

CDI	1,1-Carbonyldiimidazole
DCM	Dichloromethane
DIPEA	*N*,*N*-Diisopropylethylamine
DMAP	4-Dimethylaminopyridine
DMF	*N*,*N*-dimethylformamide
EDC·HCl	1-Ethyl-3-(3-dimethylaminopropyl)carbodiimide · hydrogen chloride
HOBt	Hydroxybenzotriazole
TCA	Trichloroacetic acid
THF	Tetrahydrofuran
Boc	Tert-butyloxycarbonyl protecting group
DMSO	Dimethyl sulfoxide

General procedures

All **synthesis products were characterised** using a Bruker Avance-III 700 MHz spectrometer with a 16.4 T superconducting magnet. Deuterated solvents (DMSO-d_6 from Sigma-Aldrich, 99.9% or acetone-d_6 from Acros Organics, 99.8%) were used for recording NMR spectra. All spectra were recorded with TopSpin 1.3 software and calibrated using the solvent signal.

For **identification of the atomic composition** the compounds were dissolved in respective solvents or solvent mixtures in a way that final solution concentration was in the order of 1 mM. 1 ml of prepared solution was spiked with 0.1 ml in-house prepared calibrant solution, which contained ions with the following exact m/z values: $C_{16}H_{36}N^+$ (m/z = 242.28423); $C_{19}H_{29}N_4PF_3^+$ (m/z = 401.20765); $C_{26}H_{45}N_7P_2Cl^+$ (m/z = 552.28947); $C_{26}H_{64}N_{13}P_4^+$ (m/z = 682.43526); $C_{44}H_{82}N_{13}P_4^+$ (m/z = 916.57611).

ESI-HRMS spectra were obtained on a hybrid Varian J-320 triple quadrupole mass spectrometer coupled with Varian 910-FT-ICR-MS. Solutions were infused into mass spectrometer using a flow rate of 3-5 ml/min. Modified nano-ESI source was used for ionization. Ionization conditions were following – nebulizing gas was not used; drying gas (N_2) pressure 15

psi at 200 °C, spray needle voltage 1800-2000 V, shield voltage 300 V; capillary voltage 40 V. Mass range of ions selected by quadrupole were guided into FT-ICR cell. Pressure in analyzer region was in order of 10^{-10} torr. Typical ADC rate of analyzer was 4 MHz, transient length: 2048 K. Varian OMEGA software was used for analyzing the spectra.

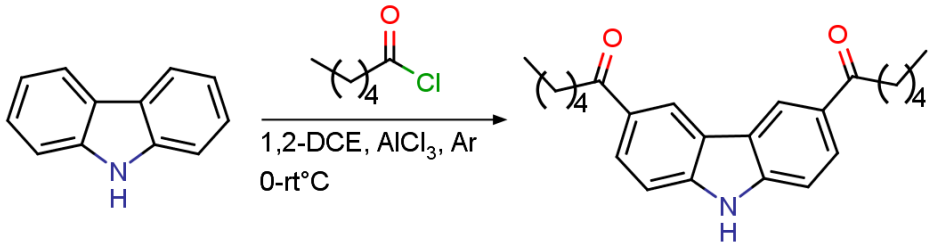
Melting points were recorded using a Büchi B-540 apparatus with open capillaries.

All **starting materials and solvents** used in synthesis were acquired from commercial sources (Sigma-Aldrich, Acros, Alfa Aesar, Fluka) with at least 97% purity and used as received. Dry solvents were prepared by filtering the solvent through a glass column packed with 3 Å molecular sieves into a pre-dried round-bottom flask supplied with additional 3 Å molecular sieves. The flasks were closed with a rubber septum and supplied with an argon-filled balloon and stored for at least 72 h before use.

Column **chromatography** was carried out on silica gel (pore size 60 Å, 230−400 mesh). Thin layer chromatography (TLC) was done using Macherey-Nagel Alugram Xtra Sil-G TLC plates with a 254 nm fluorescent marker.

All inert gases used in this work were of at least 5.0 purity. Water used for synthesis was acquired from a MilliQ Advantage A10 system.

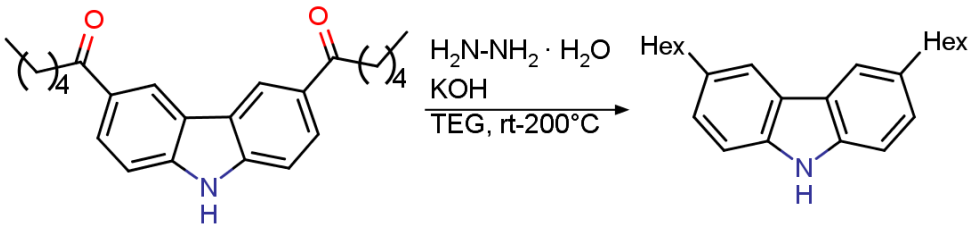
Synthesis of 3,6-dihexanoylcarbazole



Carbazole (6 g, 0.04 mol) was weighed into a round-bottom flask alongside $AlCl_3$ (11 g, 0.08 mol). The substances were dissolved in dry 1,2-dichloroethane (50 mL) and the flask was equipped with a big magnetic stirring rod, a rubber septum and a balloon filled with argon. The flask was placed into an ice bath and cooled. Hexanoyl chloride (11.5 mL, 0.08 mol) was added

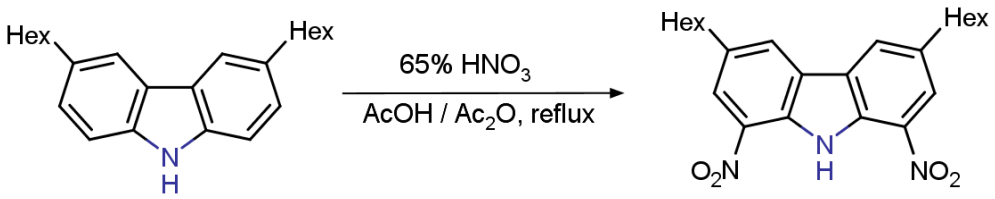
dropwise via syringe injection through the septum. After adding the reactant, the ice bath was removed and the mixture was stirred at room temperature overnight. The following day, the reaction was quenched with cold water. The organic layer was extracted, repeatedly washed with MilliQ grade water, dried with $MgSO_4$ and concentrated under reduced pressure. The obtained solid was purified by repeated recrystallization from methanol, affording the purified product (11.6 g, 0.03 mol, 89%) as a white solid.

Synthesis of 3,6-dihexylcarbazole (Huang-Minlon modification of the Wolff-Kishner reaction)



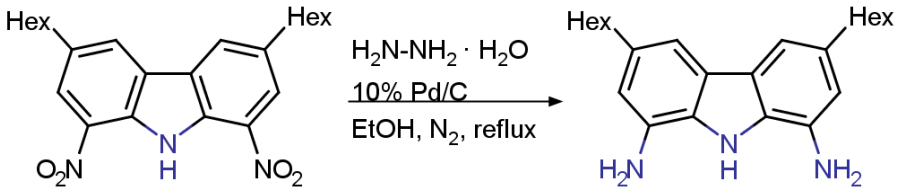
3,6-dihexanoylcarbazole (10.1 g, 0.03 mol) was weighed into a round-bottom flask alongside KOH (4.68 g, 0.08 mol). 50-60% hydrazine hydrate (6.06 mL) and triethylene glycol (50 mL) were added. The round-bottom flask was equipped with a condenser and thermometer using a 2-neck adapter. The mixture was heated to 128°C for 1.5 h. Then, the condenser was removed and the apparatus prepared for distillation. The temperature was raised to 200°C and the mixture heated for 3 h. After cooling the reaction mixture to room temperature, 5% $HCl_{(aq)}$ was used to precipitate the product and neutralize the alkaline environment. The precipitate was collected on a glass Bucher funnel and washed with MilliQ grade water (500 mL) and ice-cold methanol (10 mL) affording the purified product as a white solid (7.32 g, 0.02 mol, 78%).

Synthesis of 1,8-dinitro-3,6-dihexylcarbazole



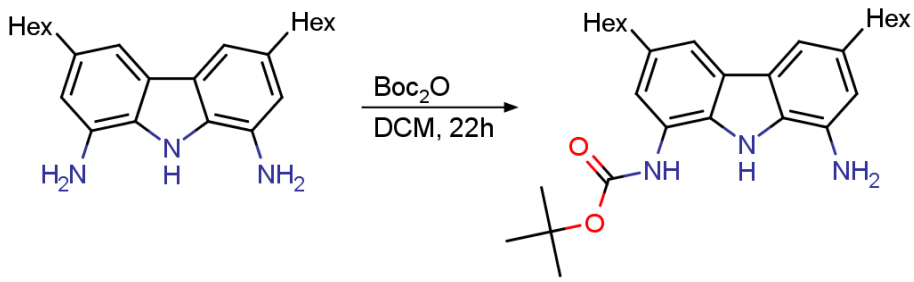
3,6-dihexylcarbazole (7.3 g, 0.02 mol) was weighed into a round-bottom flask. Acetic acid (28.7 mL) and acetic acid anhydride (21.3 mL) were poured into the flask. The mixture was placed into an ice bath and 65% $HNO_{3(aq)}$ (10.1 mL) was added. The ice bath was removed and the mixture refluxed. After 1 h, the hot mixture was poured onto a glass Buchner funnel and the obtained precipitate washed first with boiling acetic acid, then with a small amount of cold water and then with DMF. 1,8-dinitro-3,6-dihexylcarbazole (4.41 g, 0.01 mol, 48%) was obtained as a bright yellow solid.

Synthesis of 1,8-diamino-3,6-dihexylcarbazole



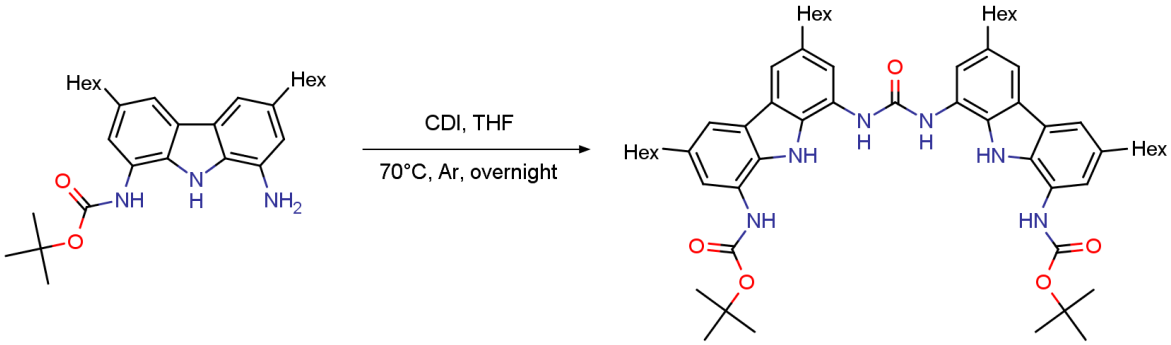
1,8-dinitro-3,6-dihexylcarbazole (4.4 g, 0.01 mol) was weighed into a round-bottom flask alongside 10% Pd/C (0.98 g) and ethanol (90 mL). The flask was supplied with a condenser, closed with a rubber septum and supplied with a N_2 filled balloon. Then, 50-60% hydrazine hydrate (25 mL) was injected dropwise to the mixture through the septum. The reaction mixture was refluxed overnight. The following day, the mixture was filtered hot on a glass Buchner funnel. The obtained Pd/C was allowed to cool and was then washed with ethanol. The filtrate was concentrated under reduced pressure and the obtained solid washed with hexane. 1,8-diamino-3,6-dihexylcarbazole (1.76 g, 0.01 mol, 47%) was obtained as an off-white solid.

Synthesis of (mono)boc-protected 1,8-diamino-3,6-dihexylcarbazole



1,8-diamino-3,6-dihexylcarbazole (1.14 g, 3.1 mmol) was weighed into a round-bottom flask and dissolved in dichloromethane (60 mL). The flask was placed into an ice bath and liquid boc-anhydride (10.1 mL) was added dropwise over the course of 1 h by using a syringe pump. The mixture was stirred at room temperature for 22 h. The crude product contained a mixture of unreacted starting material, mono- and di-boc protected compounds (this equilibrium could not be shifted in repeated experiments). Isocratic (15% ethyl acetate/hexane) column chromatography was used to purify the mixture and collect the product (467 mg, 1.0 mmol, 32%) as an off-white solid.

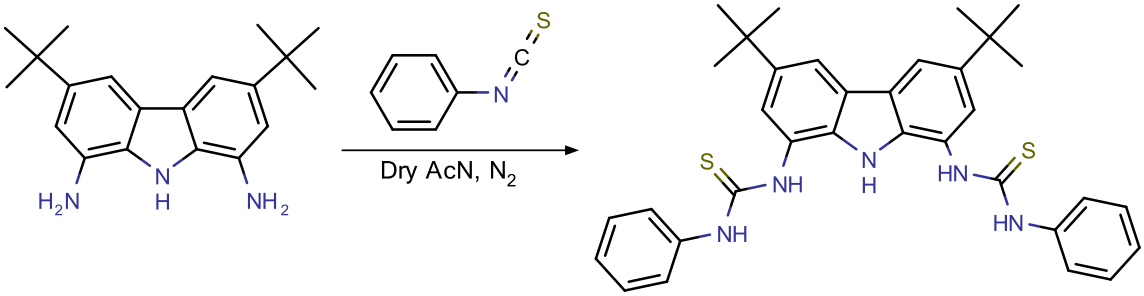
Synthesis of 1,3-bis(3,6-dihexyl-8-(tert-butoxycarbnylamino)-carbazole-1-yl)urea (CZ13)



Mono-boc protected 1,8-diamino-3,6-dihexylcarbazole (200 mg, 0.43 mmol) was weighed into a round-bottom flask alongside CDI (52 mg, 0.32 mmol). Dry THF (30 mL) was added, the flask was equipped with a condenser, sealed with a rubber septum and equipped with an argon filled balloon. The mixture was stirred overnight at 70°C. After disappearance of the starting material (monitored by TLC) the mixture was concentrated. The crude product was washed with MilliQ grade water and diethyl ether to afford **CZ13** (100 mg, 0.1 mmol, 49%) as a white solid.

Mp: decomposed above 229°C. ^{1}H NMR (700.1 MHz, DMSO-d_6, +25 °C) δ: 11.09 (br s, 2H), 9.42 (br s, 2H), 7.63 (br s, 2H), 7.53 (br s, 6H), 2.68 – 2.65 (m, 8H), 1.67 – 1.61 (m, 8H), 1.46 (s, 18H), 1.35 – 1.28 (m, 24H), 0.88 – 0.87 (m, 12H). ^{13}C NMR (176.0 MHz, DMSO-d_6, +25 °C) δ: 153.5, 153.3, 132.7, 132.5, 130.6, 129.5, 124.1, 123.7, 116.4, 113.7, 78.8, 35.7, 35.6, 31.8, 31.3, 31.2, 28.5, 28.4, 28.2, 22.1, 14.0. ESI-FT-ICR (+) (*m/z*): 956.64977 calculated for $[C_{59}H_{84}N_6O_5]^+$, (*m/z)* found 956.64922, solvent 1:1 DCM/methanol (0.1% HCOOH).

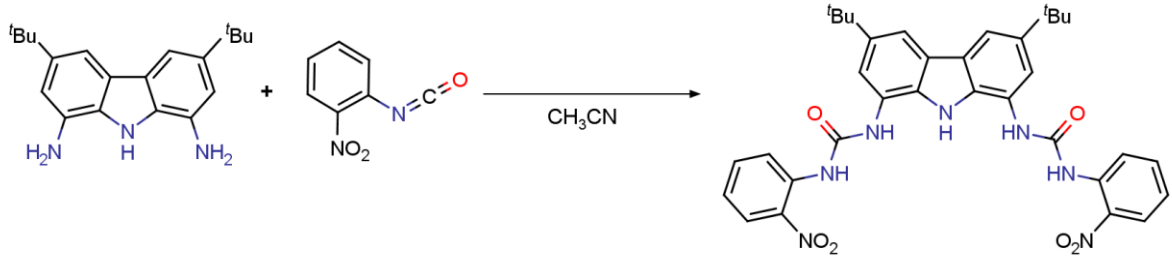
Synthesis of CZ05



3,6-di-tert-butyl-carbazole (108 mg, 0.35 mmol) was dissolved in dry acetonitrile. Phenyl isothiocyanate (200 µl, 1.67 mmol) was added. The reaction mixture was stirred overnight under N_2 atmosphere at room temperature. Then, the formed precipitate was filtered and washed with hexane. After drying, the crude product was purified with column chromatography using 0-30% ethyl acetate/hexane affording the purified **CZ05** (119 mg, 0.2 mmol, 59%).

Mp: 141°C. ^{1}H NMR (700.1 MHz, DMSO-d_6, +25 °C) δ: 10.30 (*bs*, carb. NH, 1H), 9.88 (*bs*, NH, 2H), 9.74 (*bs*, NH, 2H), 8.02 (d, 2H), 7.55-7.45 (m, 6H), 7.35-7.27 (m, 4H), 7.11-7.06 (m, 2H), 1.38 (s, 18H) ppm. ^{13}C NMR (176.0 MHz, DMSO-d_6, +25 °C) δ: 180.2, 142.0, 140.0, 133.4, 128.8, 125.0, 124.8, 123.2, 120.9, 114.3, 34.9, 32.2 ppm. ESI FT-ICR (*m/z*): 578.24176 calculated for $[C_{34}H_{36}N_5S_2]^{-1}$, (*m/z*) found 578.24184, solvent acetonitrile.

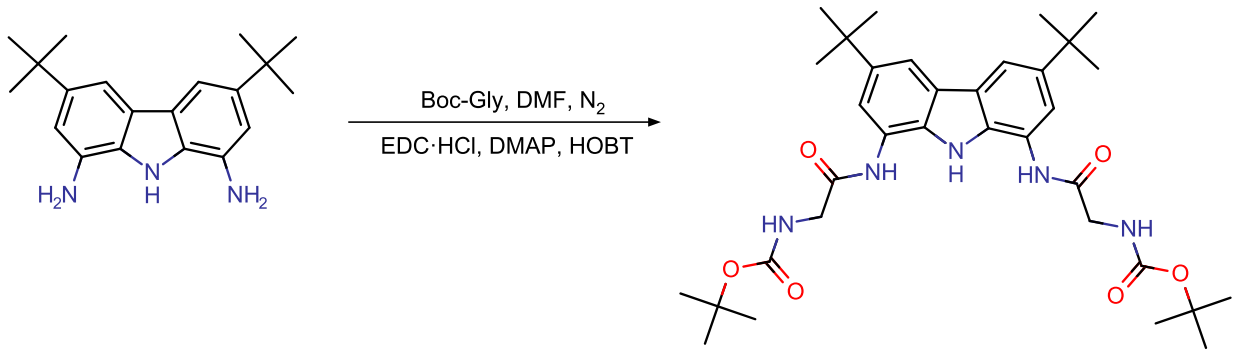
Synthesis of CZ06



1,8-diamino-3,6-di-tert-butyl-carbazole (52 mg, 0.17 mmol) was dissolved in dry acetonitrile (10 mL). Then, 2-nitrophenyl isocyanate (69 mg, 0.42 mmol) was added and the mixture was stirred at room temperature for 5 h. The reaction mixture was concentrated under reduced pressure and hexane was added to the oily crude product to precipitate the desired compound. The solid was filtered and washed with hexane to obtain **CZ06** (50 mg, 0.08 mmol, 47%) as a yellow solid.

Mp: decomposed above 172°C. ^{1}H NMR (700.1 MHz, acetone-d_6, +25 °C) δ: 9.97 (br s, 2H), 9.21 (br s, 1H), 8.79 – 8.77 (m, 2H), 8.16 – 8.15 (m, 2H), 8.02 (s, 2H), 7.68 – 7.66 (m, 2H), 7.53 – 7.52 (m, 2H), 7.19 – 7. 17 (m, 2H), 1.45 – 1.48 (m, 20H). ^{13}C NMR (176.0 MHz, acetone-d_6, +25 °C) δ: 152.7, 142.5, 136.4, 136.3, 135.4, 125.5, 125.4, 121.8, 121.6, 34.4, 31.5, 31.4, 31.4. ESI-FT-ICR (+) (*m/z*): 660.2541 calculated for $[C_{34}H_{35}N_7O_6+Na]^+$, (*m/z)* found 660.25411, solvent 1:1 DCM/methanol (0.1% HCOOH).

Synthesis of CZ07



1-8-diamino-3,6-di-tert-butyl-carbazole (100 mg, 0.32 mmol) was dissolved in 6 ml dry DMF. DMAP (100 mg, 0.82 mmol), EDC·HCl (157 mg, 0.82 mmol), HOBT (92 mg, 0.68 mmol) and

boc-protected glycine (119 mg, 0.68 mmol) were added into the reaction mixture. The flask was stirred overnight at room temperature under N_2 atmosphere. Then the reaction was quenched using 15 ml MilliQ-grade water. The crude mixture was filtered and washed with water. 135 mg of crude reaction product was collected to be purified with column chromatography (0-25% THF/hexane). However, the reaction product had decomposed during eluting. Using preparative TLC, a small amount of pure **CZ07** was collected for characterisation.

^{1}H NMR (700.1 MHz, DMSO-d6, +25 °C) δ: 10.00 (bs, NH, 3H), 7.96 (s, ArH, 2H), 7.66 (s, ArH, 2H), 7.08 (t, NH, 2H), 3.90 (s, CH_2, 4H), 1.415 (s, CH_3, 18H), 1.38 (s, CH_3, 18H) ppm. ^{13}C NMR (176.0 MHz, DMSO-d6, +25 °C) δ: 168.80, 156.31, 142.02, 131.09, 124.67, 122.43, 117.39, 113.25, 78.55, 44.09, 34.87, 32.24, 28.65 ppm. ESI FT-ICR *(m/z)* 658.33769 calculated for $[C_{34}H_{49}N_5O_6Cl]^{-1}$, *(m/z)* found 658.33789, solvent methanol.

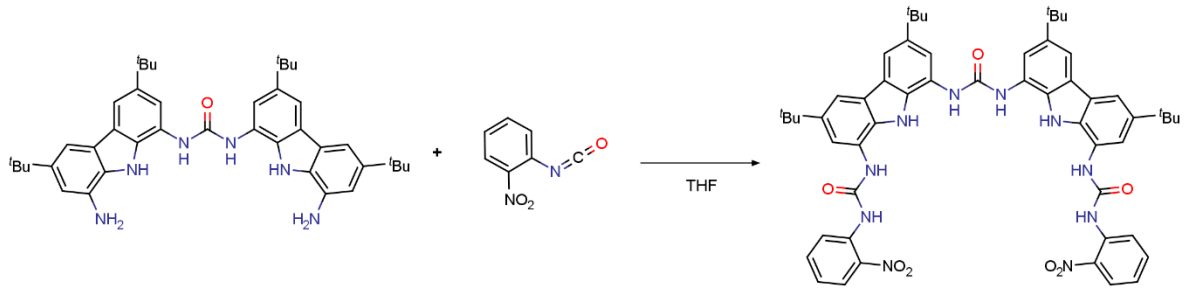
Synthesis of CZ09

1,3-bis(8-amino-3,6-di-tert-butyl-9H-carbazol-1-yl)urea **(CZ16)** (0.05 g, 0.08 mmol), lauric acid (0.04 g, 0.08 mmol), EDC·HCl (0.07 g, 0.19 mmol), HOBt (0.03 g, 0.19 mmol) and DMAP (0.02 g, 0.19 mmol) were dissolved in dry DMF (4 mL) under a nitrogen atmosphere. The reaction mixture was stirred for 48 h at room temperature. After disappearance of starting material (monitored by TLC), the reaction mixture was quenched in water (50 mL). The formed precipitate was filtered and washed with water (50 mL). The crude product was purified by column chromatography eluting with 7-9% ethyl acetate in hexane to get compound **CZ09** (0.05 g, 0.05 mmol, 64%) as a brown solid.

Mp: decomposed above 201°C. ^{1}H NMR (700.1 MHz, DMSO-d_6, +25 °C) δ: 10.10 (br s, 2H, amide NH), 10.00 (br s, 2H, carb. NH), 8.89 (br s, 2H, urea NH), 7.95 (s, 2H, CH-5), 7.93 (s, 2H,

CH-4), 7.68 (s, 2H, CH-7), 7.53 (s, 2H, CH-2), 2.40-2.35 (m, 4H, -CO-C$\underline{H}_2$), 1.61-1.56 (m, 4H, -CO-CH$_2$-C$\underline{H}_2$), 1.42 (s, 18H, *t-butyl*-C$\underline{H}_{3a}$ or C$\underline{H}_{3b}$), 1.40 (s, 18H, *t-butyl*-C$\underline{H}_{3a}$ or C$\underline{H}_{3b}$), 1.37-1.20 (m, 32H, (C$\underline{H}_2$)$_8$), 0.91-0.81 (m, 6H, -CH$_2$-C$\underline{H}_3$). ^{13}C NMR (176.0 MHz, DMSO-d$_6$, +25 °C) δ: 171.5 (amide $\underline{C}$O), 153.7 (urea $\underline{C}$O), 141.8 (C-3), 141.5 (C-6), 131.2 (C-12), 130.5 (C-9), 124.6 (C-10), 124.5 (C-11), 123.0 (C-1), 122.6 (C-8), 116.5 (C-7), 116.1 (C-2), 112.1 (C-9), 111.9 (C-4), 36.1 (-CO-$\underline{C}$H$_2$), 34.5 (*t-butyl*-$\underline{C}_a$ or $\underline{C}_b$), 34.4 (*t-butyl*-$\underline{C}_a$ or $\underline{C}_b$), 31.9, 31.8, 31.3, 29.0, 29.0, 28.9, 28.8, 28.7, 28.7, 25.2, 22.1, 13.9 (-CH$_2$-$\underline{C}$H$_3$). ESI-FT-ICR (-) (*m/z*): 1007.74711 calculated for [C$_{65}$H$_{95}$N$_6$O$_3$-H]$^-$, (*m/z)* found 1007.74706, solvent ~ 0.01% DMSO:methanol.

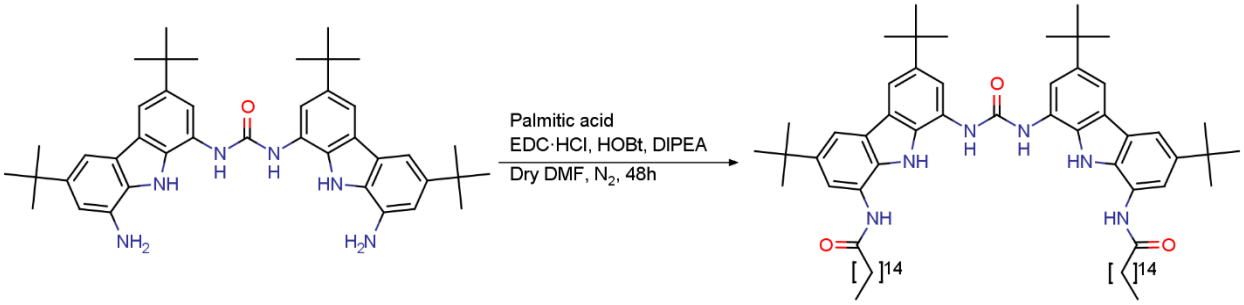
Synthesis of CZ12



1,3-bis(8-amino-3,6-di-tert-butyl-9H-carbazol-1-yl)urea **(CZ16)** (200 mg, 0.3 mmol) was dissolved in dry THF (30 mL). The solution was stirred at room temperature and 2-nitrophenyl isocyanate (127 mg, 0.77 mmol) was added. After 5 h, the reaction mixture was concentrated under reduced pressure. Hexane was added to the crude product to form a yellow solid that was filtered. After washing the solid with additional hexane, **CZ12** (212 mg, 0.22 mmol, 70%) was obtained as a yellow solid.

Mp: 242.6 – 243.8°C. ^{1}H NMR (700.1 MHz, DMSO-*d*$_6$, +25 °C) δ: 10.09 (br s, 2H), 9.85 (br s, 2H), 9.73 (br s, 2H), 8.95 (br s, 2H), 8.34 – 8.33 (m, 2H), 8.05 – 8.04 (m, 2H), 7.97 – 7.95 (m, 4H), 7.54 – 7.51 (m, 4H), 7.35 – 7.33 (m, 2H), 7.09 – 7.07 (m, 2H), 1.42 – 1.37 (m, 36H). ^{13}C NMR (176.0 MHz, acetone-d$_6$, +25 °C) δ: 142.2, 136.2, 134.8, 125.7, 125.3, 124.9, 122.1, 121.3, 116.6, 115.9, 112.7, 34.4, 31.5, 31.4. ESI-FT-ICR (+) (*m/z*): 973.47192 calculated for [C$_{55}$H$_{61}$N$_{10}$O$_7$+H]$^+$, (*m/z)* found 973.47170, solvent 1:1 DCM/methanol (0.1% HCOOH).

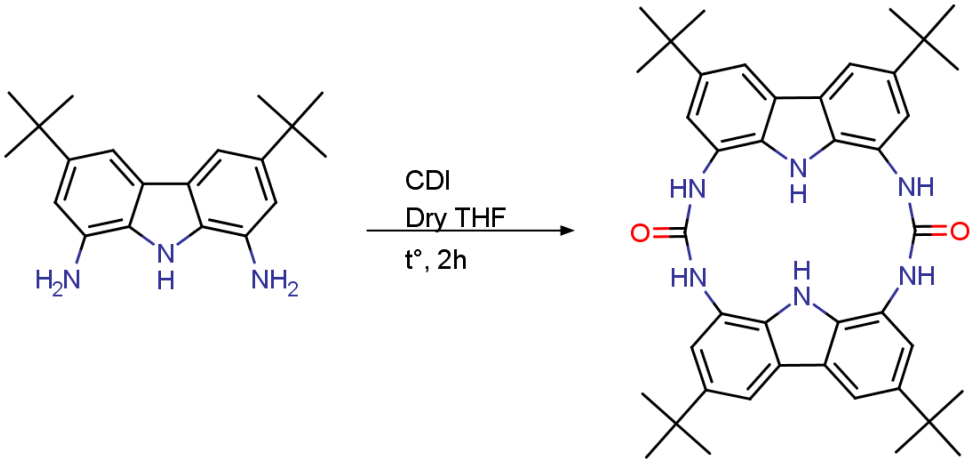
Synthesis of CZ14



1,3-bis(8-amino-3,6-di-tert-butyl-9H-carbazol-1-yl)urea **(CZ16)** (61 mg, 0.01 mmol), palmitic acid (61 mg, 0.24 mmol), EDC·HCl (54 mg, 0.28 mmol), HOBt (38 mg, 0.28 mmol) were dissolved in dry DMF (5 mL) under a nitrogen atmosphere. DIPEA (37 mg, 0.28 mmol) was added dropwise to the solution. The mixture was stirred at room temperature for 48 h. After disappearance of starting materials (as monitored by TLC), the reaction was quenched with $NaHCO_3$ solution. This precipitated the product, which was filtered and washed with methanol (20 mL) to obtain **CZ14** (80 mg, 0.07 mmol, 73%) as a white solid.

Mp: decomposed above 180°C. ^{1}H NMR (700.1 MHz, DMSO-d_6, +25 °C) δ: 10.15 (br s, 2H), 10.00 (br s, 2H), 8.90 (br s, 2H), 7.88 (s, 2H), 7.85 (s, 2H), 7.74 (br s, 2H), 7.58 (br s, 2H), 2.40 (m, 4H), 1.61 (m, 4H), 1.43 (s, 16H), 1.41 (s, 16H), 1.21 – 1.19 (m, 48H), 0.85 (t, J = 7 Hz, 6H). ^{13}C NMR (176.0 MHz, DMSO-d_6, +25 °C) δ: 171.9, 154.1, 142.1, 141.9, 131.5, 130.8, 124.9, 123.1, 116.4, 112.8, 112.2, 34.9, 34.8, 32.3, 32.2, 31.7, 29.5, 29.4, 29.4, 29.3, 29.2, 29.2, 29.1, 25.7, 22.5, 14.4. ESI-FT-ICR (+) (*m/z*): 1121.88687 calculated for $[C_{73}H_{112}N_6O_3+H]^+$, (*m/z)* found 1121.88677, solvent 1:1 DCM/methanol (0.1% HCOOH).

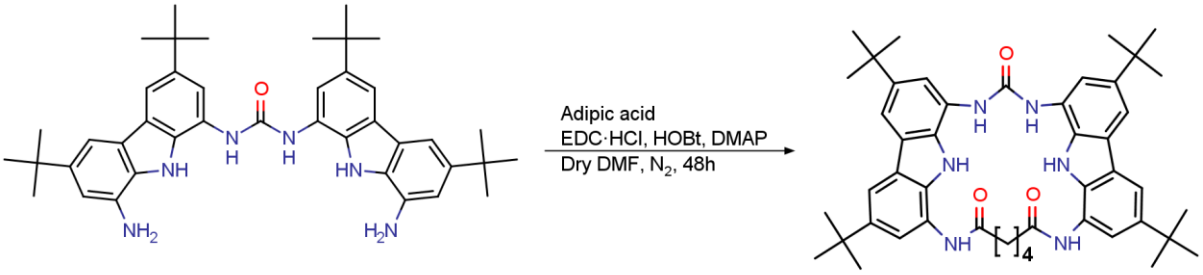
Synthesis of MC01



1,8-diamino-3,6-di-tert-butyl-carbazole (0.08 g, 0.24 mmol), was dissolved in dry THF (4 mL), then CDI (0.10 g, 0.43 mmol) was added. The reaction mixture was stirred at reflux temperature for 2 h. After disappearance of the starting material (monitored by TLC), the reaction mixture was cooled and concentrated under reduced pressure. The obtained solid was quenched in H_2O (100 mL) and the solution extracted with ethyl acetate (50 mL). The ethyl acetate layer was concentrated under reduced pressure. The crude product was purified by column chromatography eluting with 1% methanol in DCM to obtain compound **MC01** (0.07 g, 0.10 mmol, 83%) as an off-white solid.

Mp: decomposed above 300°C. ^{1}H NMR (700.1 MHz, DMSO-d_6, +25 °C) δ: 9.87 (br s, 2H, carb. N<u>H</u>), 9.20 (br s, 4H, amide N<u>H</u>), 8.01 (d, J = 1.4 Hz, 4H, C<u>H</u>-4), 7.16 (d, J = 2.1 Hz, 4H, C<u>H</u>-2), 1.44 (s, 36H, *t-butyl*-C<u>H</u>$_3$). ^{13}C NMR (176.0 MHz, DMSO-d_6, +25 °C) δ: 153.7 (urea <u>C</u>O), 143.2 (<u>C</u>-3), 134.4 (<u>C</u>-6), 126.9 (<u>C</u>-5), 123.9 (<u>C</u>-1), 117.2 (<u>C</u>-2), 113.5 (<u>C</u>-4), 34.9 (*t-butyl*-<u>C</u>), 32.3 (*t-butyl*-<u>C</u>H$_3$). ESI-FT-ICR (+) (*m/z*): 669.39225 calculated for $[C_{42}H_{48}N_6O_2+H]^+$, (*m/z)* found 669.39217, solvent methanol (0.1% HCOOH).

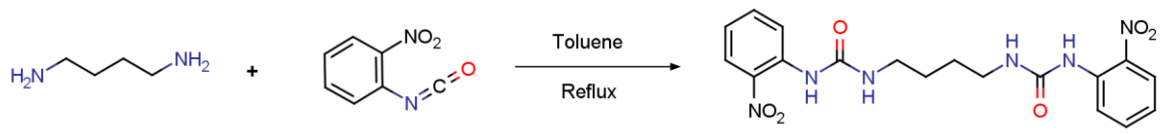
Synthesis of MC04



1,3-bis(8-amino-3,6-di-tert-butyl-9H-carbazol-1-yl)urea **(CZ16)** (0.06 g, 0.09 mmol), adipic acid (0.01 g, 0.09 mmol), EDC·HCl (0.05 g, 0.28 mmol), HOBt (0.04 g, 0.28 mmol) and DMAP (0.02 g, 0.19 mmol) were dissolved in dry DMF (5 mL). The reaction mixture was stirred for 48 h at room temperature. After disappearance of the starting material (monitored by TLC) the reaction mixture was quenched in water (50 mL). The formed precipitate was filtered and washed with water (50 mL). The crude product was purified by column chromatography eluting with 1-2% methanol in DCM to get compound **MC04** (0.05 g, 0.07 mmol, 71%) as an off-white solid.

Mp: 311.0-313.4°C. ^{1}H NMR (700.1 MHz, DMSO-d_6, +25 °C) δ: 10.17 (br s, 2H, amide NH), 9.35 (br s, 2H, carb NH), 8.90 (br s, 2H, urea NH), 8.01 (d, J = 1.4 Hz, 2H, CH-5), 7.90 (d, J = 1.4 Hz, 2H, CH-4), 7.84 (d, J = 1.4 Hz, 2H, CH-2), 7.40 (d, J = 1.4 Hz, 2H, CH-7), 2.58-2.52 (m, 4H, -CO-CH$_2$), 1.93-1.91 (m, 4H, -CO-CH$_2$-CH$_2$), 1.45 (s, 18H, *t-butyl*-CH$_{3a}$ or CH$_{3b}$), 1.42 (s, 18H, *t-butyl*-CH$_{3a}$ or CH$_{3b}$). ^{13}C NMR (176.0 MHz, DMSO-d_6, +25 °C) δ: 171.6 (amide CO), 153.6 (urea CO), 142.6 (C-3 or C-6), 142.4 (C-3 or C-6), 131.8 (C-9), 130.4 (C-12), 125.0 (C-11), 124.1 (C-10), 123.3 (C-1), 122.4 (C-8), 117.1 (C-7), 115.4 (C-2), 113.3 (C-5), 111.4 (C-4), 35.3 (CO-CH$_2$), 34.6 (*t-butyl*-C$_a$ or C$_b$), 34.4 (*t-butyl*-C$_a$ or C$_b$), 32.0 (*t-butyl*-CH$_{3a}$ or CH$_{3b}$), 31.8 (*t-butyl*-CH$_{3a}$ or CH$_{3b}$), 24.4 (-CO-CH$_2$-CH$_2$). ESI-FT-ICR (+) (*m/z*): 755.46432 calculated for $[C_{47}H_{58}N_6O_3+H]^+$, (*m/z*) found 755.46429, solvent methanol (0.1% HCOOH).

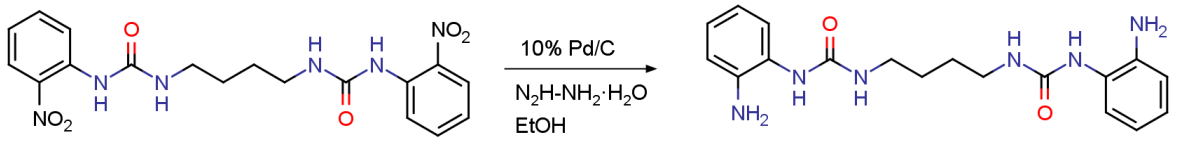
Synthesis of U01



To a stirred solution of 2-nitrophenyl isocyanate (820 mg, 4.99 mmol) in 50 mL dry toluene, 1,4-diaminobutane (219 mg, 2.49 mmol) was added dropwise at room temperature. The mixture was refluxed for 3 h and then cooled to room temperature. The formed yellow crude product precipitated from the solution and was filtered. The obtained solid was washed with diethyl ether to afford **U01** (900 mg, 2.16 mmol, 87%) as a light yellow solid.

Mp: 257.3 - 259.2°C. ^{1}H NMR (700.1 MHz, DMSO-d_6, +25 °C) δ: 9.34 (br s, 2H), 8.33 (d, J = 8.4 Hz, 2H), 8.05 (dd, J = 1.4 & 8.4 Hz, 2H), 7.66 - 7.58 (m, 2H), 7.54 (br s, 2H), 7.15 - 7. 09 (m, 2H), 3.13 - 3.12 (m, 4H), 1.49 (s, 4H). ^{13}C NMR (176.0 MHz, DMSO-d_6, +25 °C) δ: 154.2, 136.6, 136.0, 135.0, 125.3, 121.9, 121.2, 39.2, 26.9. ESI-FT-ICR (+) (*m/z*): 465.10759 calculated for $[C_{18}H_{20}N_6O_6+K]^+$, (*m/z*) found 455.10783, solvent ~ 0.01% DMSO:methanol.

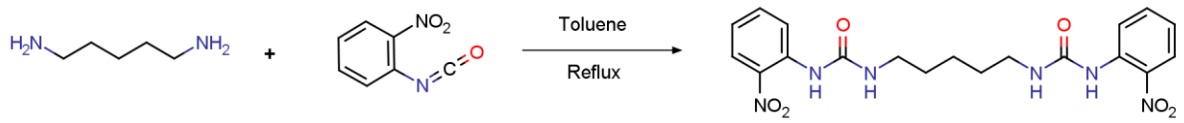
Synthesis of U02



To a stirred solution of **U01** (750 mg, 1.80 mmol) in ethanol (70 mL), 10% Pd/C (200 mg) and 50-60% hydrazine hydrate (1.5 mL) were added. The mixture was refluxed for 18 h. After full conversion of starting material (monitored by TLC), the mixture was cooled and the formed precipitate was filtered. The solids were transferred into another flask and DMF (25 mL) was added. The Pd/C was filtered and the product precipitated from DMF by addition of water. The obtained solid product was filtered and washed with water and methanol to afford **U02** (350 mg, 0.98 mmol, 54%) as an off-white solid.

Mp: 193.1 - 194.5°C. ^{1}H NMR (700.1 MHz, DMSO-d_6, +25 °C) δ: 7.47 (br s, 2H), 7.26 (d, J = 7.7 Hz, 2H), 6.80 - 6.73 (m, 2H), 6.69 - 6.68 (m, 2H), 6.53 - 6.51 (m, 2H), 6.16 - 6.15 (m, 2H), 4.67 (br s, 4H), 3.09 - 3.08 (m, 4H), 1.45 (s, 4H). ^{13}C NMR (176.0 MHz, DMSO-d_6, +25 °C) δ: 155.9, 140.5, 125.7, 123.7, 123.2, 116.8, 115.8, 39.0, 27.4. ESI-FT-ICR (+) (*m/z*): 357.20390 calculated for $[C_{18}H_{24}N_6O_2+H]^+$, (*m/z*) found 357.20324, solvent ~ 0.01% DMSO:methanol.

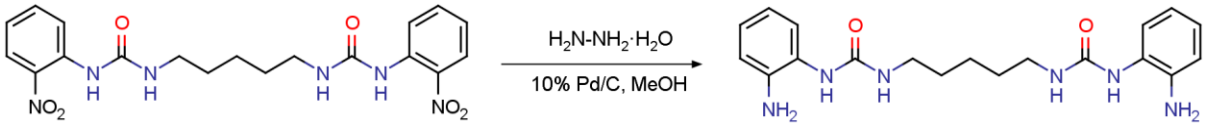
Synthesis of U03



To a stirred solution of 1,5-diaminopentane (200 mg, 1.96 mmol) in toluene (70 mL) 2-nitrophenyl isocyanate (803 mg, 4.90 mmol) was added dropwise at room temperature. The mixture was refluxed for 3 h. After full conversion of starting material (monitored by TLC), the mixture was cooled to room temperature. The formed solid was filtered and washed with diethyl ether to afford **U03** (700 mg, 1.63 mmol, 83%) as a light yellow solid.

Mp: 195.7 - 196.4°C. ^{1}H NMR (700.1 MHz, DMSO-d_6, +25 °C) δ: 9.34 (br s, 2H), 8.32 (d, J = 8.4 Hz, 2H), 8.03 (dd, J = 1.4 & 9.4 Hz, 2H), 7.65 - 7.58 (m, 2H), 7.54 (br s, 2H), 7.11 - 7.10 (m, 2H), 3.12 - 3.10 (m, 4H), 1.49 - 1.45 (m, 4H), 1.36 - 1.35 (m, 2H).^{13}C NMR (176.0 MHz, DMSO-d_6, +25 °C) δ: 154.6, 137.1, 136.5, 135.5, 125.8, 122.3, 121.7, 40.4, 29.6, 24.2. ESI-FT-ICR (+) (*m/z*): 431.16791 calculated for $[C_{19}H_{22}N_6O_6+H]^+$, (*m/z*) found 431.16746, solvent ~ 0.01% DMSO:methanol.

Synthesis of U04

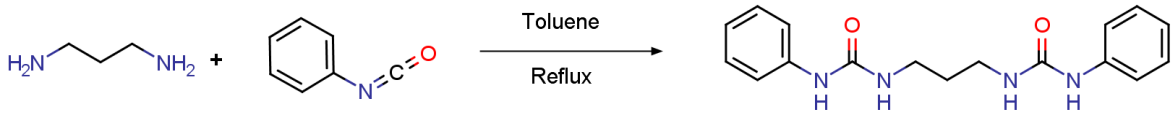


To a stirred solution of **U03** (450 mg, 1.04 mmol) in methanol (70 mL), 10% Pd/C (40 mg) and 50-60% hydrazine hydrate (1 mL) were added at room temperature. The suspension was stirred at reflux temperature for 18 h. After full conversion of starting material (monitored by TLC), the mixture was allowed to cool and the formed precipitate was filtered. The obtained solid was dissolved in DMF (50 mL) and quenched with water. The solid was filtered and washed with DCM and diethyl ether to afford **U04** (200 mg, 0.54 mmol, 52%) as an off-white solid.

Mp: 184.2 - 185.3°C. ^{1}H NMR (700.1 MHz, DMSO-d_6, +25 °C) δ: 7.47 (br s, 2H), 7.26 (dd, J = 7.9, 1.1 Hz. 2H), 6.77 (td, J = 7.7, 1.5 Hz, 2H), 6.68 (dd, J =7.8, 1.4 Hz, 2H), 6.52 (td, J = 7.7,

1.4 Hz, 2H), 6.15 (t, J = 5.6 Hz, 2H), 4.67 (br s, 4H), 3.07 (q, J = 6.74 Hz, 4H), 1.45 (quint, J =7.2 Hz, 4H), 1.32 (m, 2H). ^{13}C NMR (176.0 MHz, DMSO-d_6, +25 °C) δ: 156.3, 140.9, 126.1, 124.1, 123.6, 117.2, 116.2, 30.1, 24.3. ESI-FT-ICR (+) (*m/z*): 371.21900 calculated for $[C_{19}H_{27}N_6O_2+H]^+$, (*m/z)* found 371.21878, solvent ~ 0.01% DMSO:methanol.

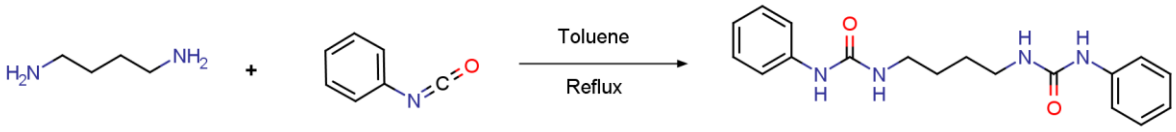
Synthesis of U05



To a stirred solution of 1,3-diaminopropane (100 mg, 1.35 mmol) in toluene (25 mL) phenyl isocyanate (369 mg, 6.21 mmol) was added at room temperature. The reaction mixture was stirred at reflux temperature for 4 h. After full conversion of starting material (monitored by TLC) the mixture was cooled to room temperature. The formed precipitate was filtered and washed with diethyl ether to afford **U05** (400 mg, 1.28 mmol, 94%) as an off-white solid.

Mp: 234.1 - 235.5°C. ^{1}H NMR (700.1 MHz, DMSO-*d*$_6$, +25 °C) δ: 8.48 (br s, 2H), 7.39 - 7.38 (m, 4H), 7.21 - 7.19 (m, 4H), 6.88 - 6.87 (m, 2H), 6.18 - 6.16 (m, 2H), 3.13 - 3.11 (m, 4H), 1.59 - 1.55 (m, 2H). ^{13}C NMR (176.0 MHz, DMSO-d_6, +25 °C) δ: 155.3, 140.6, 128.6, 120.9, 117.7, 36.5, 30.7. ESI-FT-ICR (+) (*m/z*): 313.16645 calculated for $[C_{17}H_{21}N_4O_2+H]^+$, (*m/z)* found 313.16562, solvent ~ 0.01% DMSO:methanol.

Synthesis of U06

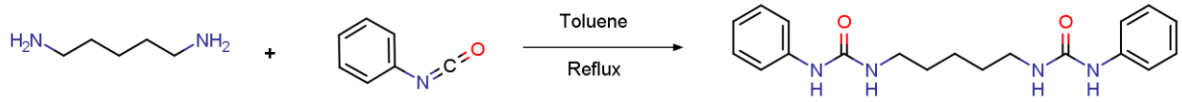


To a stirred solution of 1,4-diaminobutane (300 mg, 0.40 mmol) in toluene (80 mL) phenyl isocyanate (1.21 g, 10.2 mmol) was added at room temperature. The reaction mixture was stirred at reflux temperature for 3 h. After full conversion of starting material (monitored by TLC), the

reaction mixture was cooled. The formed precipitate was filtered and washed with diethyl ether to afford **U06** (800 mg, 2.45 mmol, 72%) as an off-white solid.

Mp: 246.1 - 247.9°C. ^{1}H NMR (700.1 MHz, DMSO-d_6, +25 °C) δ: 8.37 (br s, 2H), 7.38 - 7.37 (m, 4H), 7.21 - 7.19 (m, 4H), 6.88 - 6.86 (m, 2H), 6.13 - 6.12 (m, 2H), 3.10 - 3.09 (m, 4H), 1.45 - 1.44 (m, 4H). ^{13}C NMR (176.0 MHz, DMSO-d_6, +25 °C) δ: 155.2, 140.6, 128.6, 120.9, 117.6, 38.8, 27.3. ESI-FT-ICR (+) (*m/z*): 327.18210 calculated for $[C_{18}H_{22}N_4O_2+H]^+$, (*m/z)* found 327.18151, solvent ~ 0.01% DMSO:methanol.

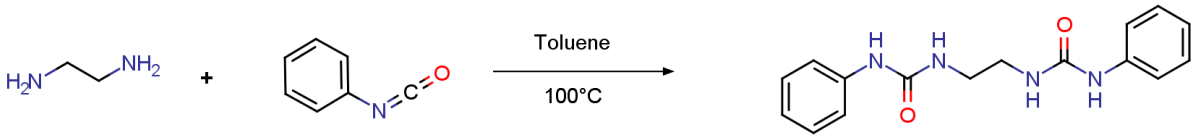
Synthesis of U07



To a stirred solution of 1,5-diaminopentane (300 mg, 2.94 mmol) in toluene (80 mL) phenyl isocyanate (1.0 g, 8.82 mmol) was added at room temperature. The reaction mixture was stirred at reflux temperature for 3 h. After full conversion of starting material (monitored by TLC), the reaction mixture was cooled. The formed precipitate was filtered and washed with diethyl ether to afford **U07** (890 mg, 2.61 mmol, 89%) as an off-white solid.

Mp: 213.1 - 214.8°C. ^{1}H NMR (700.1 MHz, DMSO-d_6, +25 °C) δ: 8.36 (br s, 2H), 7.38 - 7.37 (m, 4H), 7.21 - 7.19 (m, 4H), 6.88 - 6.86 (m, 2H), 6.12 - 6.10 (m, 2H), 3.09 - 3.06 (m, 4H), 1.47 - 1.43 (m, 4H), 1.33 - 1.32 (m, 2H). ^{13}C NMR (176.0 MHz, DMSO-d_6, +25 °C) δ: 155.2, 140.6, 128.6, 120.9, 117.6, 39.01, 29.5, 23.8. ESI-FT-ICR (+) (*m/z*): 341.19775 calculated for $[C_{19}H_{24}N_4O_2+H]^+$, (*m/z)* found 341.19718, solvent ~ 0.01% DMSO:methanol.

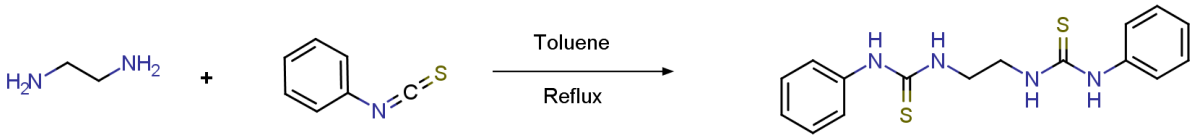
Synthesis of U08



To a stirred solution of 1,2-diaminoethane (150 mg, 2.68 mmol) in toluene (70 mL) phenyl isocyanate (883 mg, 7.0 mmol) was added at room temperature. The reaction mixture was stirred at reflux temperature for 12 h. After full conversion of starting material (monitored by TLC) the reaction mixture was cooled to room temperature. The obtained precipitate was filtered and washed with diethyl ether to afford **U08** (690 mg, 2.31 mmol, 92%) as an off-white solid.

Mp: decomposed above 263°C. NMR data was unobtainable due to solubility restrictions. ESI-FT-ICR (+) (*m/z*): 299.15025 calculated for $[C_{18}H_{22}N_4O_2+H]^+$, (*m/z)* found 299.15012, solvent ~ 0.01% DMSO:methanol.

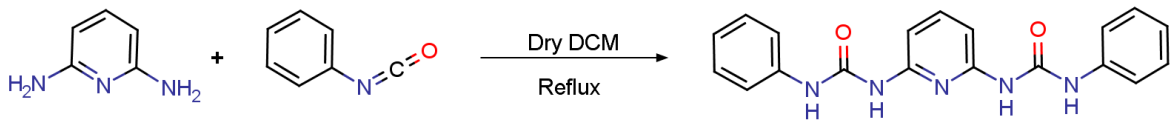
Synthesis of U09



To a stirred solution of ethylenediamine (100 mg, 2.0 mmol) in toluene (50 mL), phenyl isothiocyanate (825 mg, 6.0 mmol) was added at room temperature. The reaction mixture was stirred at reflux temperature for 3 h. After full conversion of the starting material (monitored by TLC) the reaction mixture was cooled to room temperature. The formed solid was filtered and washed with diethyl ether to afford **U09** (500 mg, 1.51 mmol, 83%) as an off-white solid.

Mp: 210.6 – 212.5°C. ^{1}H NMR (700.1 MHz, DMSO-d_6, +25 °C) δ: 9.60 (br s, 2H), 7.82 (br s, 2H), 7.39 (d, J = 7.5 Hz, 4H), 7.32 (t, J = 7.5 Hz, 4H), 7.12 (t, J = 7.3 Hz, 2H), 3.71 (br s, 4H). ^{13}C NMR (176.0 MHz, DMSO-d_6, +25 °C) δ: 180.6, 138.9, 128.7, 124.4, 123.3, 43.3. ESI-FT-ICR (+) (*m/z*): 331.10456 calculated for $[C_{16}H_{18}N_4S_2+H]^+$, (*m/z)* found 331.10452, solvent ~ 0.01% DMSO:methanol.

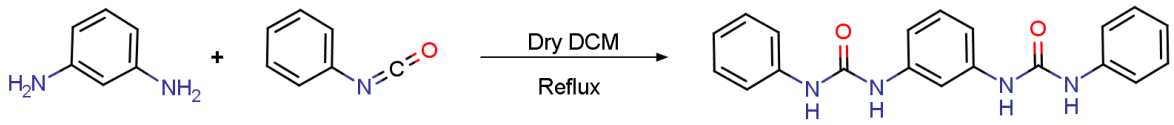
Synthesis of U10



To a stirred solution of 2,6-diaminopyridine (200 mg, 1.83 mmol) in dry DCM (25 mL) phenyl isocyanate (480 mg, 4.03 mmol) was added dropwise. The reaction mixture was stirred at reflux temperature for 2 h. After full conversion of starting material (monitored by TLC) the solution was cooled and the formed solid filtered. After washing with DCM, **U10** (150 mg, 0.43 mmol, 23%) was obtained as an off-white solid.

Mp: decomposed above 300°C. ^{1}H NMR (700.1 MHz, DMSO-d_6, +25 °C) δ: 9.84 (br s, 2H), 9.22 (br s, 2H), 7.68 - 7.65 (m, 1H), 7.59 - 7.58 (m, 4H), 7.33 - 7.31 (m, 4H), 7.13 (d, J = 7.7 Hz, 2H), 7.04 - 7.02 (m, 2H). ^{13}C NMR (176.0 MHz, DMSO-d_6, +25 °C) δ: 151.9, 150.8, 140.3, 139.1, 128.8, 122.5, 119.1, 104.8. ESI-FT-ICR (+) (*m/z*): 348.14605 calculated for $[C_{19}H_{17}N_5O_2+H]^+$, (*m/z)* found 348.14552, solvent ~ 0.01% DMSO:methanol.

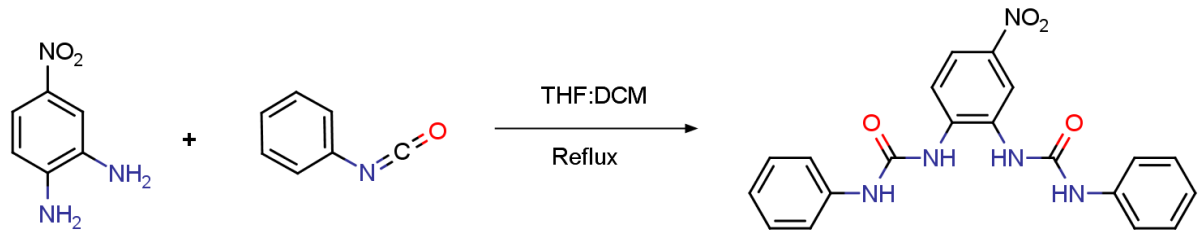
Synthesis of U11



To a stirred solution of 1,3-diaminobenzene (500 mg, 4.62 mmol) in dry DCM (80 mL) phenyl isocyanate (1.38 g, 11.6 mmol) was added dropwise. The reaction mixture was stirred at reflux temperature for 16 h. After full conversion of starting material (monitored by TLC), the solution was cooled to room temperature. The formed solid was filtered and washed with DCM to afford **U11** (1.60 g, 4.62 mmol, 99%) as an off-white solid.

Mp: decomposed above 300°C. ^{1}H NMR (700.1 MHz, DMSO-d_6, +25 °C) δ: 8.70 (br s, 2H), 8.60 (br s, 2H), 7.67 - 7.66 (m, 1H), 7.46 - 7.45 (m, 4H), 7.29 - 7.27 (m, 4H), 7.17 - 7.15 (m, 1H), 7.08 – 7.07 (m, 2H), 6.98 – 6.96 (m, 2H). ^{13}C NMR (176.0 MHz, DMSO-d_6, +25 °C) δ: 152.4, 140.2, 139.7, 129.1, 128.9, 128.8, 121.8, 118.1, 111.7, 107.8. ESI-FT-ICR (+) (*m/z*): 347.15025 calculated for $[C_{20}H_{18}N_4O_2+H]^+$, (*m/z)* found 347.15025, solvent ~ 0.01% DMSO:methanol.

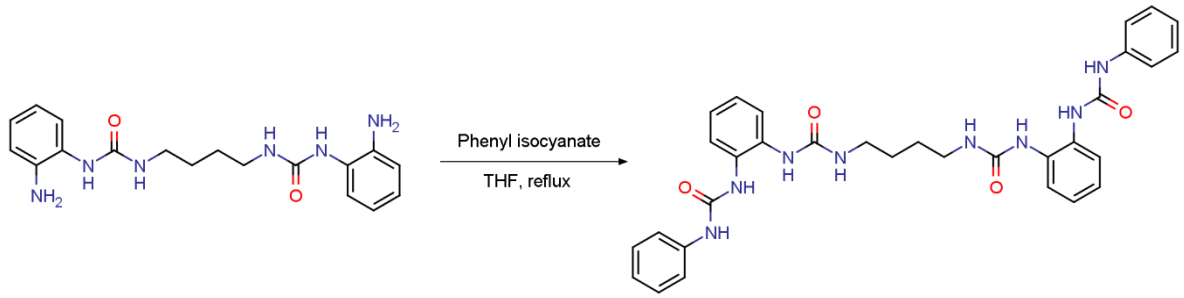
Synthesis of U14



To a stirred solution of 1,2-diamino-4-nitrobenzene (20 mg, 1.3 mmol) in a mixture of THF (8 mL) and DCM (15 mL) phenyl isocyanate (311 mg, 2.61 mmol) was added at room temperature. The reaction mixture was stirred at reflux temperature for 16 h. After full conversion of starting material (monitored by TLC) the solution was cooled to room temperature. The formed solid was filtered and washed with DCM and methanol to afford **U14** (300 mg, 0.77 mmol, 59%) as an off-white solid.

Mp: 213.4 - 214.5°C. ^{1}H NMR (700.1 MHz, DMSO-d_6, +25 °C) δ: 9.36 (br s, 1H), 9.10 (br s, 1H), 8.61 (br s, 1H), 8.42 (br s, 1H), 8.30 (br s, 1H), 8.13 (d, J = 8.4 Hz, 1H), 8.02 (d, J = 8.4 Hz, 1H), 7.51 - 7.49 (m, 4H), 7.32 - 7.31 (m, 4H), 7.02 – 7.00 (m, 2H). ^{13}C NMR (176.0 MHz, DMSO-d_6, +25 °C) δ: 153.1, 152.2, 141.8, 139.4, 139.3, 139.1, 129.3, 128.9, 128.8, 122.4, 122.2, 121.0, 120.1, 119.9, 118.4, 118.3. ESI-FT-ICR (+) (*m/z*): 414.11728 calculated for $[C_{20}H_{17}N_5O_4+Na]^+$, (*m/z)* found 414.11721, solvent ~ 0.01% DMSO:methanol.

Synthesis of U21

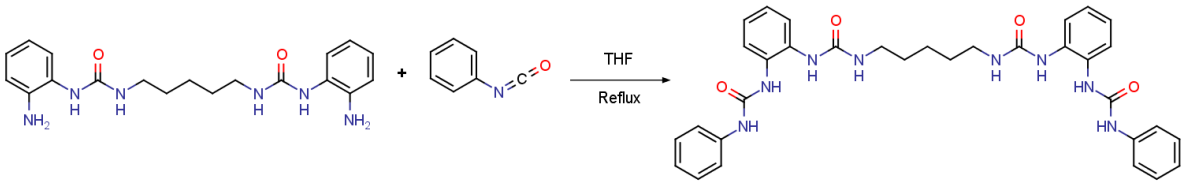


To a stirred solution of **U02** (150 mg, 0.42 mmol) in dry tetrahydrofuran (50 mL), phenyl isocyanate (150 mg, 1.26 mmol) was added. The mixture was stirred at reflux temperature for 18

h. The mixture was allowed was to cool and the formed precipitate was filtered and washed with DCM and diethyl ether to afford **U21** (180 mg, 0.30 mmol, 72%) as an off-white solid.

Mp: 204.7 - 207.1°C. ^{1}H NMR (700.1 MHz, DMSO-d_6, +25 °C) δ: 9.05 (br s, 2H), 7.99 (br s, 2H), 7.80 (br s, 2H), 7.53 - 7.45 (m, 8H), 7.27 - 7.25 (m, 4H), 7.03 - 6.93 (m, 6H), 6.55 - 6.53 (m, 2H), 3.12 (s, 4H), 1.47 (s, 4H). ^{13}C NMR (176.0 MHz, DMSO-d_6, +25 °C) δ: 155.9, 153.2, 140.0, 132.2, 130.6, 128.8, 128.7, 124.2, 123.9, 123.2, 123.1, 121.8, 121.6, 118.2, 118.1 39.9, 27.4. ESI-FT-ICR (+) (*m/z*): 595.27813 calculated for $[C_{32}H_{34}N_8O_4+H]^+$, (*m/z)* found 595.27785, solvent ~ 0.01% DMSO:methanol.

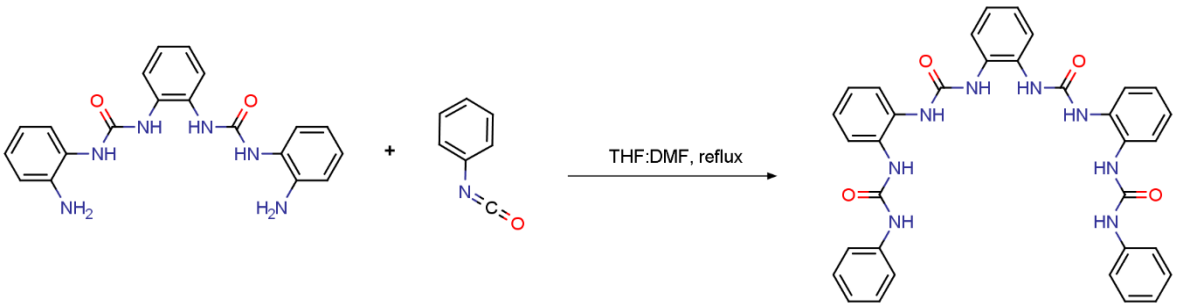
Synthesis of U22



To a stirred solution of **U04** (70 mg, 0.19 mmol) in dry tetrahydrofuran (25 mL) phenyl isocyanate (67 mg, 0.56 mmol) was added at room temperature. The mixture was stirred at reflux temperature for 17 h. The mixture was allowed to cool and the formed precipitate was filtered. The obtained solid was washed with DCM and diethyl ether to afford **U22** (90 mg, 0.15 mmol, 78%) as an off-white solid.

Mp: 189.2 - 191.3°C. ^{1}H NMR (700.1 MHz, DMSO-d_6, +25 °C) δ: 9.06 (br s, 2H), 7.99 (br s, 2H), 7.80 (br s, 2H), 7.53 - 7.45 (m, 8H), 7.27 - 7.25 (m, 4H), 7.03 - 6.94 (m, 6H), 6.52 - 6.51 (m, 2H), 3.11 - 3.08 (m, 4H), 1.47 - 1.44 (m, 4H), 1.34 - 1.32 (m, 2H). ^{13}C NMR (176.0 MHz, DMSO-d_6, +25 °C) δ: 156.3, 153.6, 140.4, 132.6, 131.1, 129.2, 124.6, 123.7, 123.6, 122.1, 118.5, 40.4, 30.0, 24.3. ESI-FT-ICR (+) (*m/z*): 631.27572 calculated for $[C_{33}H_{36}N_8O_4+Na]^+$, (*m/z)* found 631.27515, solvent ~ 0.01% DMSO:methanol.

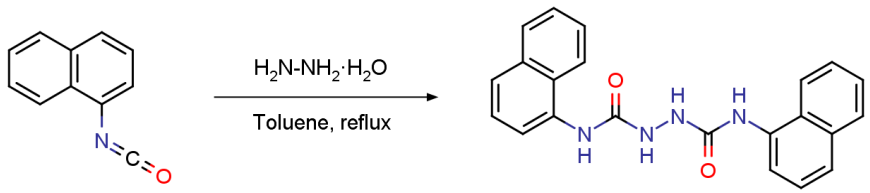
Synthesis of U23



To a stirred solution of **U16** (150 mg, 0.39 mmol) in THF (50 mL) and DMF (5 mL) phenyl isocyanate (142 mg, 1.19 mmol) was added at room temperature. The reaction mixture was stirred at reflux temperature for 3 h. After full conversion of starting material (monitored by TLC) the reaction mixture was cooled to room temperature. The formed solid was filtered and washed with THF to afford **U23** (130 mg, 0.21 mmol, 54%) as an off-white solid.

Mp: decomposed above 300°C. ^{1}H NMR (700.1 MHz, DMSO-d_6, +25 °C) δ: 9.10 (br s, 2H), 8.50 (br s, 4H), 8.48 (br s, 2H), 8.07 (br s, 2H), 7.63 - 7.57 (m, 4H), 7.53 – 7.52 (m, 2H), 7.44 - 7.43 (m, 4H), 7.26 - 7.24 (m, 4H), 7.08 - 7.01 (m, 6H), 6.96 - 6.94 (m, 2H). ^{13}C NMR (176.0 MHz, DMSO-d_6, +25 °C) δ: 154.1, 153.2, 139.8, 131.5, 131.3, 131.0, 128.8, 124.3, 124.2, 124.1, 124.0, 123.9, 123.8, 121.8, 118.1. ESI-FT-ICR (+) (*m/z*): 615.24628 calculated for $[C_{18}H_{22}N_4O_2+H]^+$, (*m/z)* found 615.24669, solvent ~ 0.01% DMSO:methanol.

Synthesis of HZ01

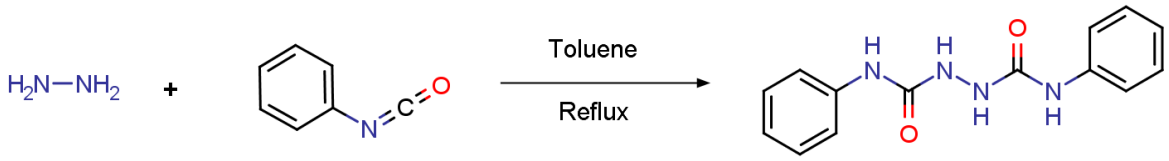


To a stirred solution of naphtyl isocyanate (200 mg, 1.18 mmol) in toluene (10 mL) 50-60% hydrazine hydrate (100 µl) was added. The reaction mixture was refluxed for 8 h. After full conversion of starting material (monitored by TLC) the reaction mixture was cooled to room

temperature. The formed precipitate from the solution was filtered and washed with diethyl ether to afford **HZ01** (300 mg, 0.81 mmol, 68%) as an off-white solid.

Mp: 235.5 – 237.5°C. ^{1}H NMR (700.1 MHz, DMSO-d_6, +25 °C) δ: 8.88 (br s, 2H), 8.37 (br s, 2H), 8.12 (d, J = 8.4 Hz, 2H), 7.92 (d, J = 8.4 Hz, 2H), 7.87 (br s, 2H), 7.66 (d, J = 8.4 Hz, 2H), 7.56 - 7.46 (m, 6H). ^{13}C NMR (176.0 MHz, DMSO-d_6, +25 °C) δ: 156.7, 134.4, 133.7, 128.3, 125.9, 125.8, 125.6, 123.5, 121.9. ESI-FT-ICR (+) (*m/z*): 371.15080 calculated for $[C_{22}H_{18}N_4O_2+H]^+$, (*m/z)* found 371.15046, solvent ~ 0.01% DMSO:methanol.

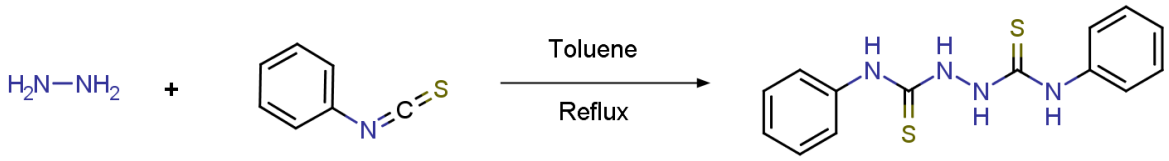
Synthesis of HZ02



To a stirred solution of hydrazine hydrate (50 mg, 1.0 mmol) in toluene (50 mL) phenyl isocyanate (353 mg, 3.0 mmol) was added at room temperature. The reaction mixture was stirred at reflux temperature for 3 h. After full conversion of starting material (monitored by TLC) the reaction mixture was cooled. The formed solid was filtered and washed with diethyl ether to afford **HZ02** (250 mg, 0.92 mmol, 92%) as an off-white solid.

Mp: 264.0 – 264.8°C. ^{1}H NMR (700.1 MHz, DMSO-d_6, +25 °C) δ: 8.75 (br s, 2H), 7.96 (br s, 2H), 7.49 - 7.48 (m, 4H), 7.26 - 7.24 (m, 4H), 6.96 - 6.94 (m, 2H). ^{13}C NMR (176.0 MHz, DMSO-d_6, +25 °C) δ: 156.0, 139.7, 128.6, 121.8, 118.5. ESI-FT-ICR (+) (*m/z*): 293.10090 calculated for $[C_{14}H_{14}N_4O_2+Na]^+$, (*m/z)* found 293.10088, solvent ~ 0.01% DMSO:methanol.

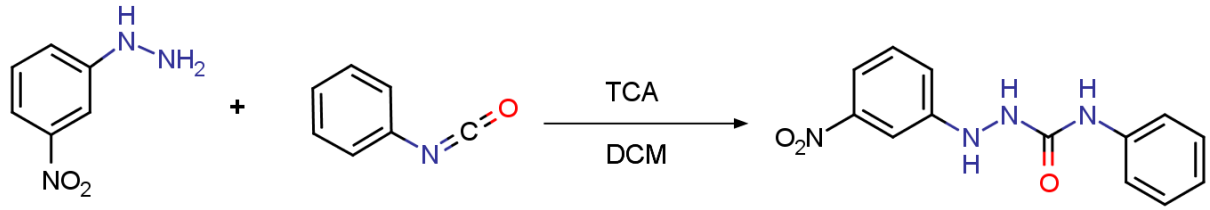
Synthesis of HZ03



To a stirred solution of 1,2-diaminoethane (100 mg, 1.66 mmol) in toluene (80 mL) phenyl isothiocyanate (575 mg, 4.16 mmol) was added at room temperature. The reaction mixture was stirred at reflux temperature for 12 h. After full conversion of starting material (monitored by TLC) the mixture was cooled to room temperature. The obtained precipitate was filtered and washed with diethyl ether to afford **HZ03** (500 mg, 1.65 mmol, 90%) as an off-white solid.

Mp: 210.6 - 212.5°C. ^{1}H NMR (700.1 MHz, DMSO-*d*$_6$, +25 °C) δ: 9.85 (br s, 2H), 9.65 (br s, 2H), 7.54 (d, J = 5.4 Hz, 4H) 7.34 (t, J = 7.5 Hz, 4H), 7.15 (t, J = 7.2 Hz, 2H). ^{13}C NMR (176.0 MHz, DMSO-d$_6$, +25 °C) δ: 181.6, 139.1, 128.1, 124.9. ^{13}C NMR (176.0 MHz, DMSO-d$_6$, +65 °C) δ: 138.8, 127.9, 124.4, 123.8. ESI-FT-ICR (+) (*m/z*): 303.07326 calculated for $[C_{14}H_{15}N_4S_2+H]^+$, (*m/z)* found 303.07320, solvent ~ 0.01% DMSO:methanol.

Synthesis of HZ05



(3-nitrophenyl)-hydrazine hydrochloride (212 mg, 1.12 mmol) was dissolved in DCM (20 mL). TCA (113 mg, 1.12 mmol) was added dropwise to the solution and then phenyl isocyanate (200 mg, 1.68 mmol) was added. After 30 minutes precipitate started forming in the solution. The reaction mixture was stirred overnight and then filtered. After washing the precipitate with DCM, **HZ05** (188 mg, 0.69 mmol, 49.9%) was obtained.

Mp: 226.4 – 228.1°C. ^{1}H NMR (700.1 MHz, DMSO-*d*$_6$, +25 °C) δ: 8.59 (bs s, 1H), 7.75 - 7.74 (m, 2H), 7.72 (d, J = 5.9 Hz, 1H), 7.70 - 7.68 (m, 1H), 7.62 (d, J = 8.4 Hz, 2H), 7.52 (td, J = 8.1, 1.7 Hz, 1H), 7.34 (dtd, J = 8.2, 2.4, 0.9 Hz, 1H), 7.26 – 7.23 (m, 2H), 6.98 (tt, J = 7.4, 1.1, 1H). ^{13}C NMR (176.0 MHz, DMSO-d$_6$, +25 °C) δ: 115.9, 150.8, 149.3, 139.7, 130.1, 128.5, 122.2, 118.9, 118.9, 118.8, 114.1, 106.9. ESI-FT-ICR (+) (*m/z*): 273.09822 calculated for $[C_{13}H_{12}N_4O_3+H]^+$, (*m/z)* found 273.09825, solvent 1:1 DCM/methanol (0.1% HCOOH).

NMR and HRMS spectra of the synthesized compounds

^{1}H NMR spectrum of compound CZ05 37

^{13}C NMR spectrum of compound CZ05 38

HRMS spectrum of compound CZ05 39

^{1}H NMR spectrum of compound CZ06 40

^{13}C NMR spectrum of compound CZ06 41

HRMS spectrum of compound CZ06 42

^{1}H NMR spectrum of compound CZ07 43

^{13}C NMR spectrum of compound CZ07 44

HRMS spectrum of compound CZ07 45

^{1}H NMR spectrum of compound CZ09 46

^{13}C NMR spectrum of compound CZ09 47

HRMS spectrum of compound CZ09 48

^{1}H NMR spectrum of compound CZ12 49

^{13}C NMR spectrum of compound CZ12 50

HRMS spectrum of compound CZ12 51

^{1}H NMR spectrum of compound CZ13 52

^{13}C NMR spectrum of compound CZ13 53

HRMS spectrum of compound CZ13 54

^{1}H NMR spectrum of compound CZ14 55

^{13}C NMR spectrum of compound CZ14 56

HRMS spectrum of compound CZ14 57

^{1}H NMR spectrum of compound MC01 58

^{13}C NMR spectrum of compound MC01 59

HRMS spectrum of compound MC01 60

^{1}H NMR spectrum of compound MC04 61

^{13}C NMR spectrum of compound MC04 62

HRMS spectrum of compound MC04 63

^{1}H NMR spectrum of compound U01 64

^{13}C NMR spectrum of compound U01 65

HRMS spectrum of compound U01 66
^{1}H NMR spectrum of compound U02 67
^{13}C NMR spectrum of compound U02 68
HRMS spectrum of compound U02 69
^{1}H NMR spectrum of compound U03 70
^{13}C NMR spectrum of compound U03 71
HRMS spectrum of compound U03 72
^{1}H NMR spectrum of compound U04 73
^{13}C NMR spectrum of compound U04 74
HRMS spectrum of compound U04 75
^{1}H NMR spectrum of compound U05 76
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^{1}H NMR spectrum of compound U07 82
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^{1}H NMR spectrum of compound U10 89
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^{1}H NMR spectrum of compound U11 92
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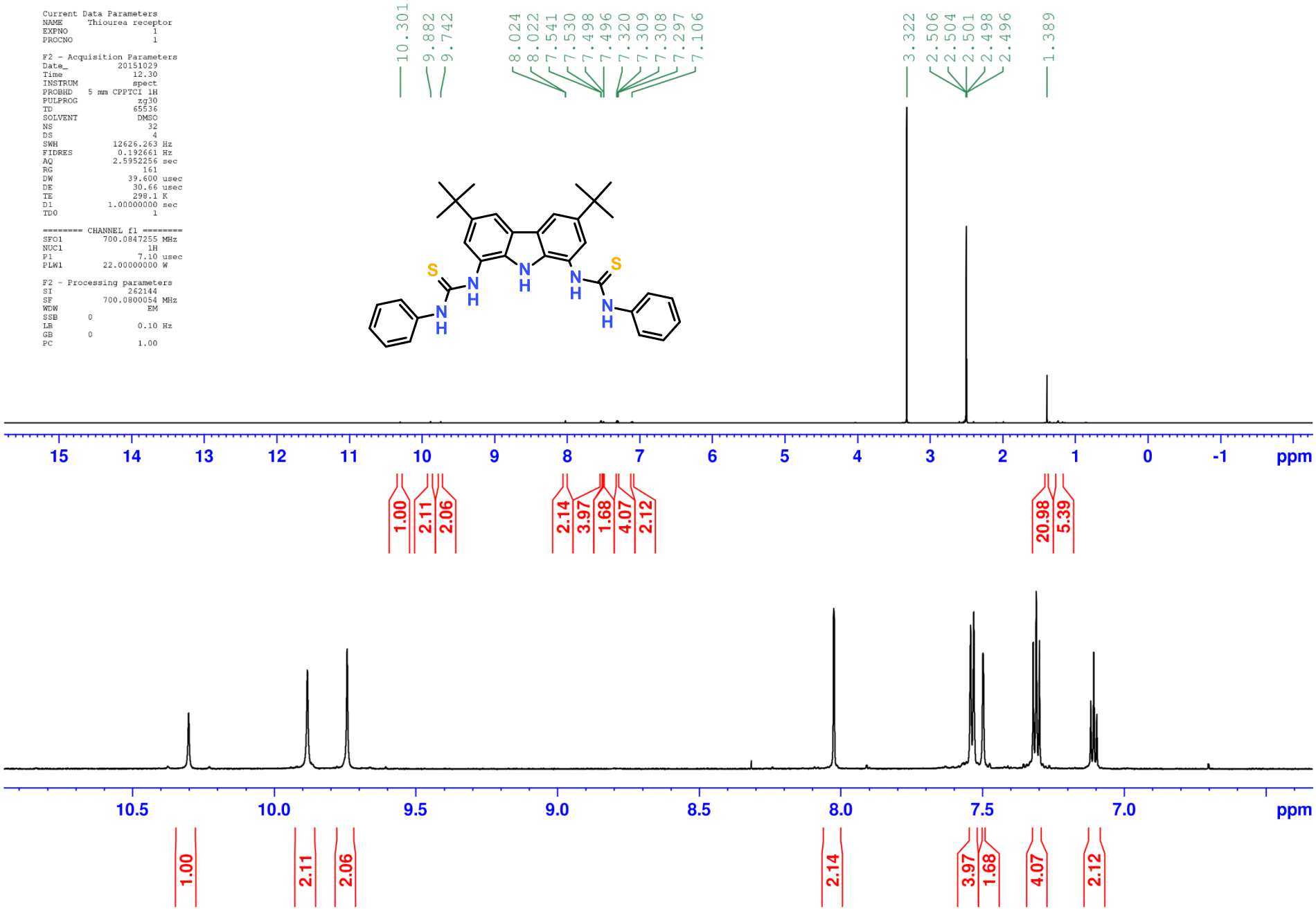
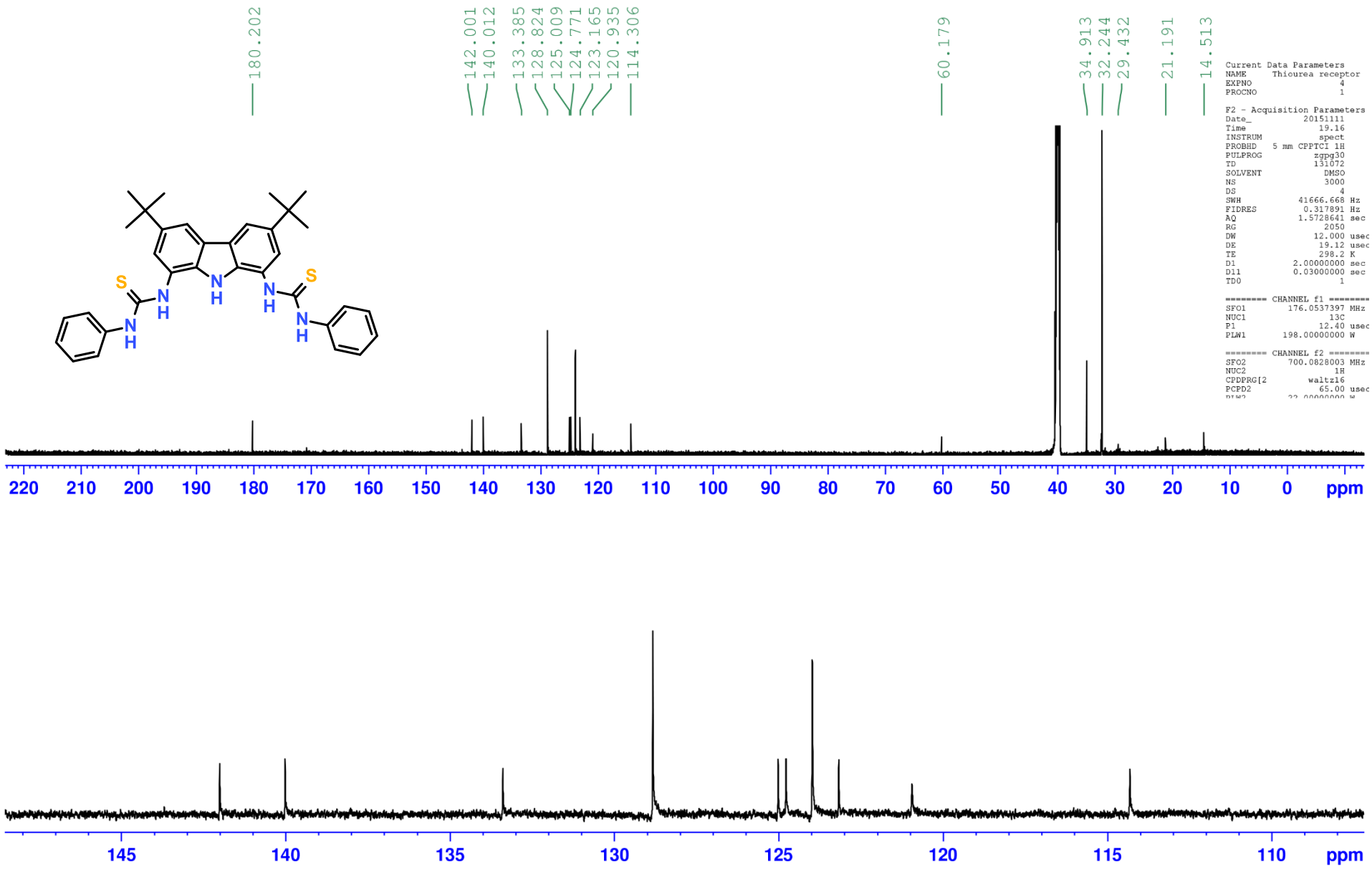
^{1}H NMR spectrum of compound U21 98
^{13}C NMR spectrum of compound U21 99
HRMS spectrum of compound U21 100
^{1}H NMR spectrum of compound U22 101
^{13}C NMR spectrum of compound U22 102
HRMS spectrum of compound U22 103
^{1}H NMR spectrum of compound U23 104
^{13}C NMR spectrum of compound U23 105
HRMS spectrum of compound U23 106
^{1}H NMR spectrum of compound HZ01 107
^{13}C NMR spectrum of compound HZ01 108
HRMS spectrum of compound HZ01 109
^{1}H NMR spectrum of compound HZ02 110
^{13}C NMR spectrum of compound HZ02 111
HRMS spectrum of compound HZ02 112
^{1}H NMR spectrum of compound HZ03 113
^{13}C NMR (+25 °C) spectrum of compound HZ03 114
^{13}C NMR (+65 °C) spectrum of compound HZ03 115
HRMS spectrum of compound HZ03 116
^{1}H NMR spectrum of compound HZ05 117
^{13}C NMR spectrum of compound HZ05 118
HRMS spectrum of compound HZ05 119

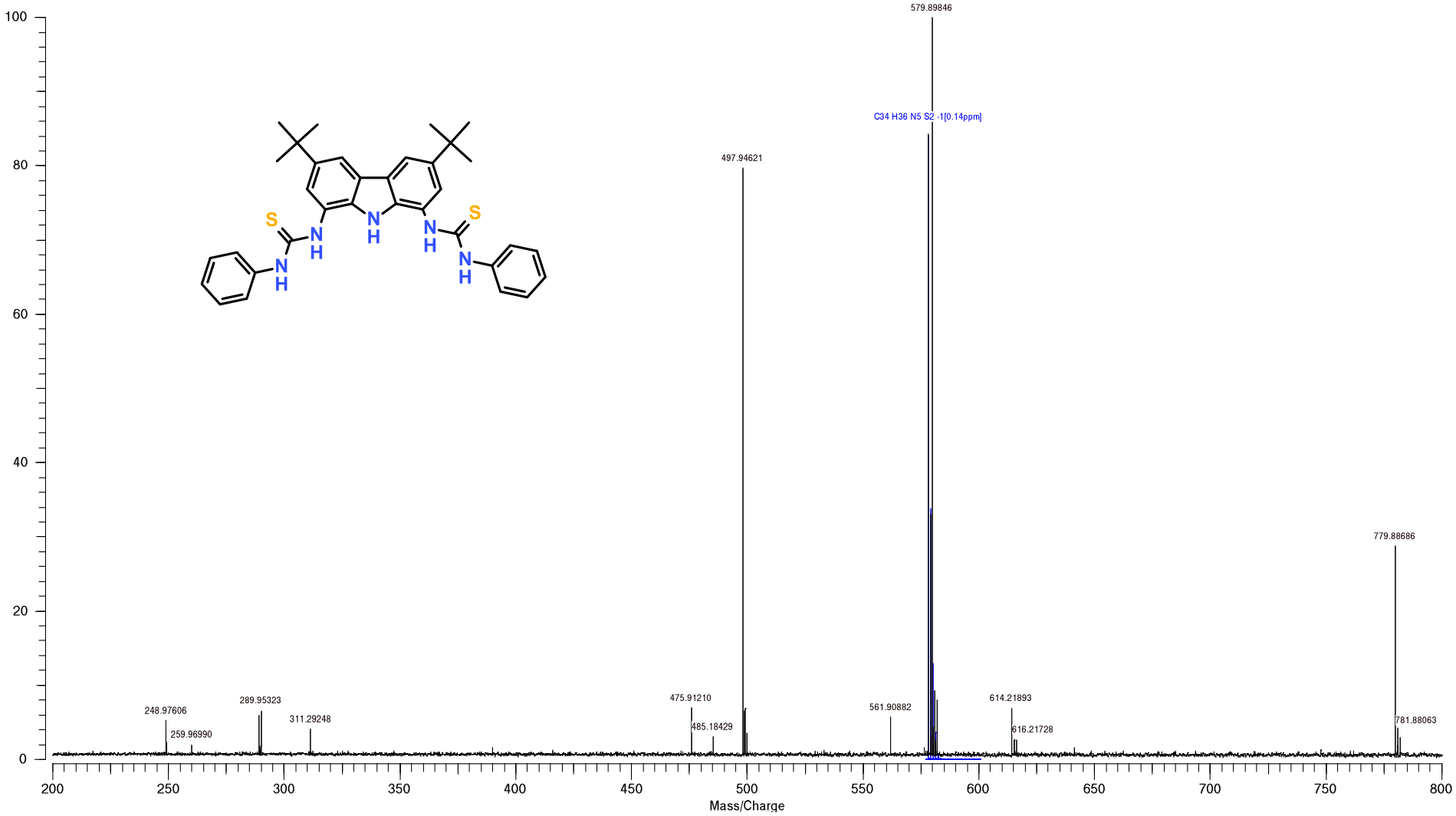
^{1}H NMR spectrum of compound CZ05



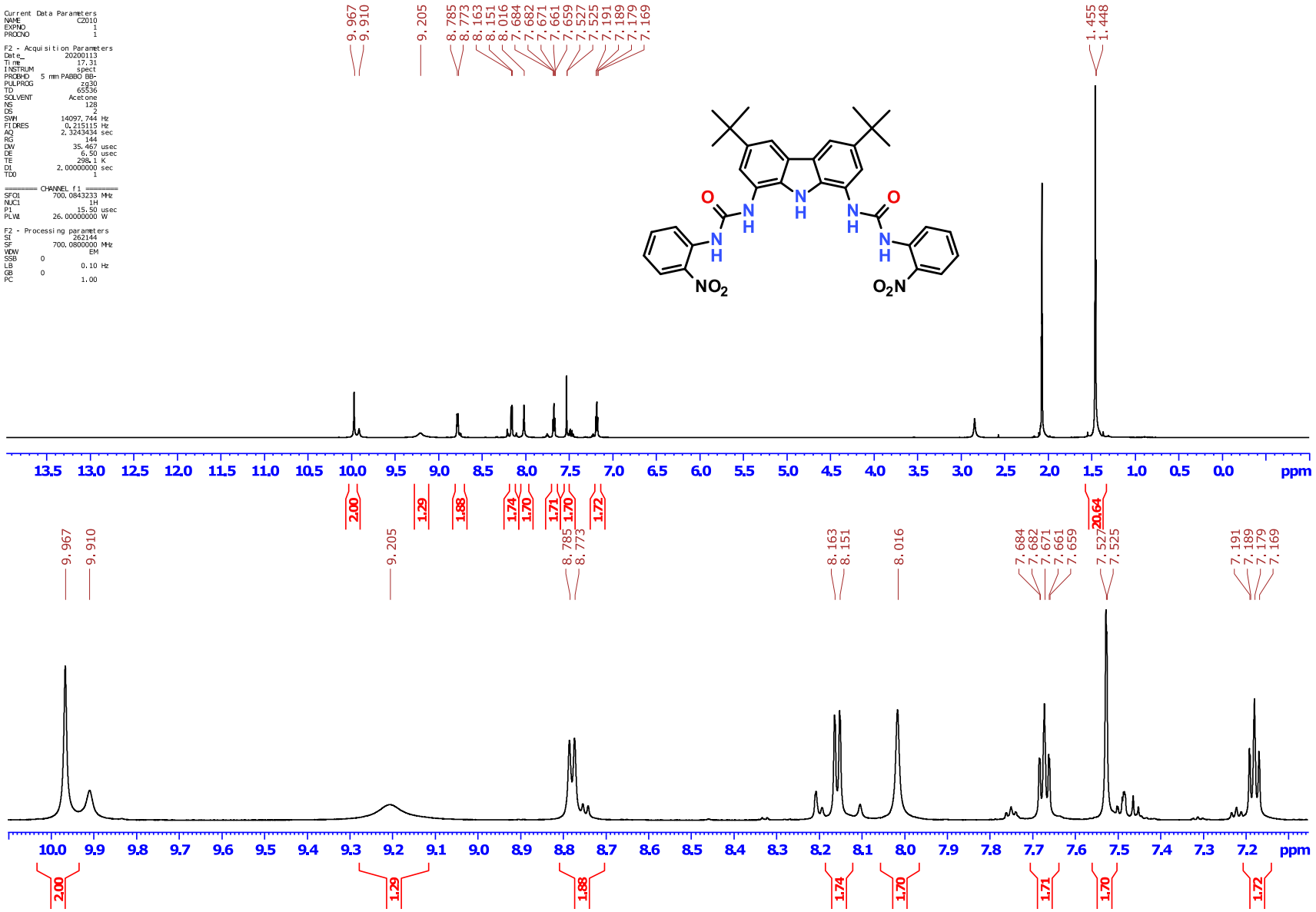
^{13}C NMR spectrum of compound CZ05



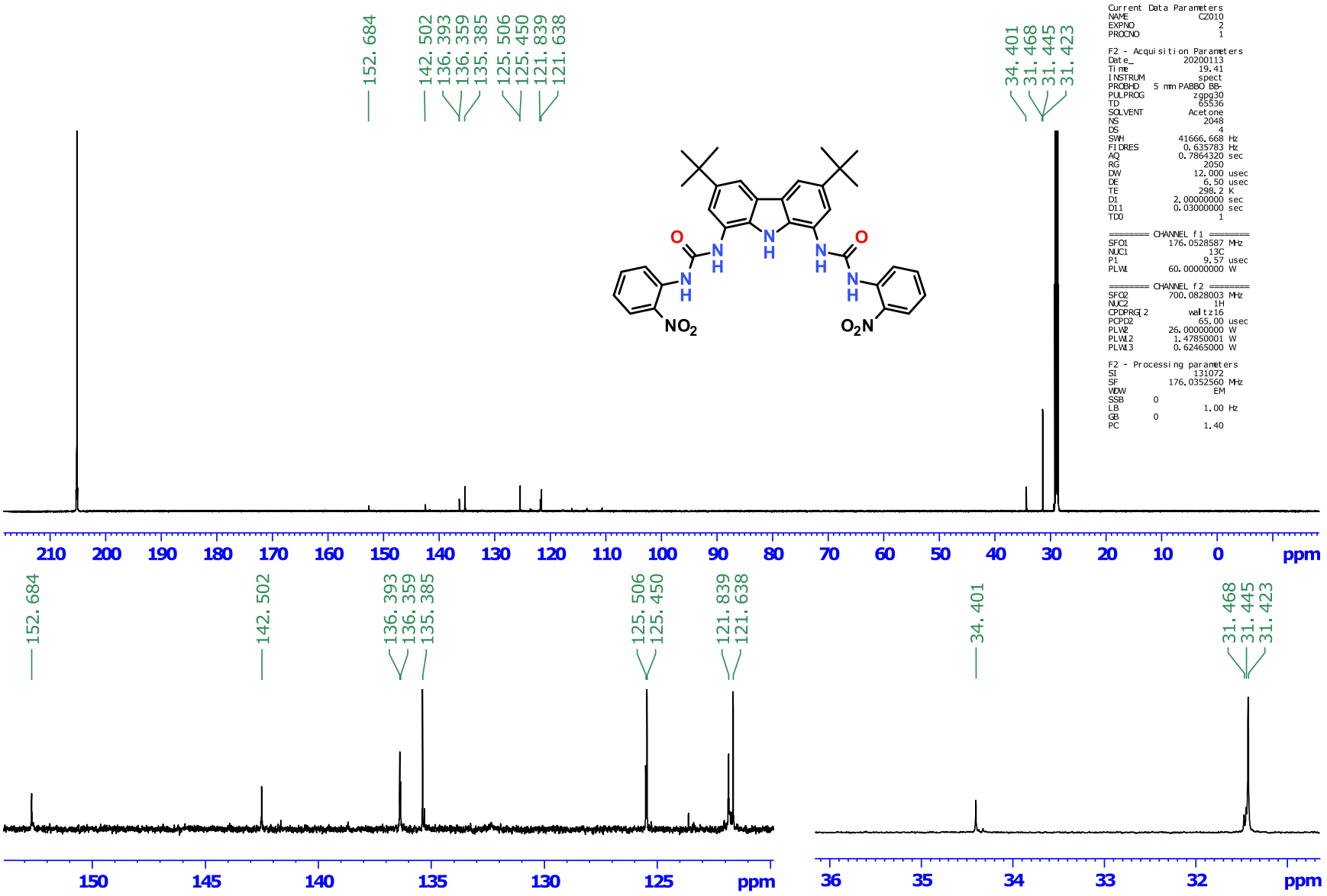
HRMS spectrum of compound CZ05



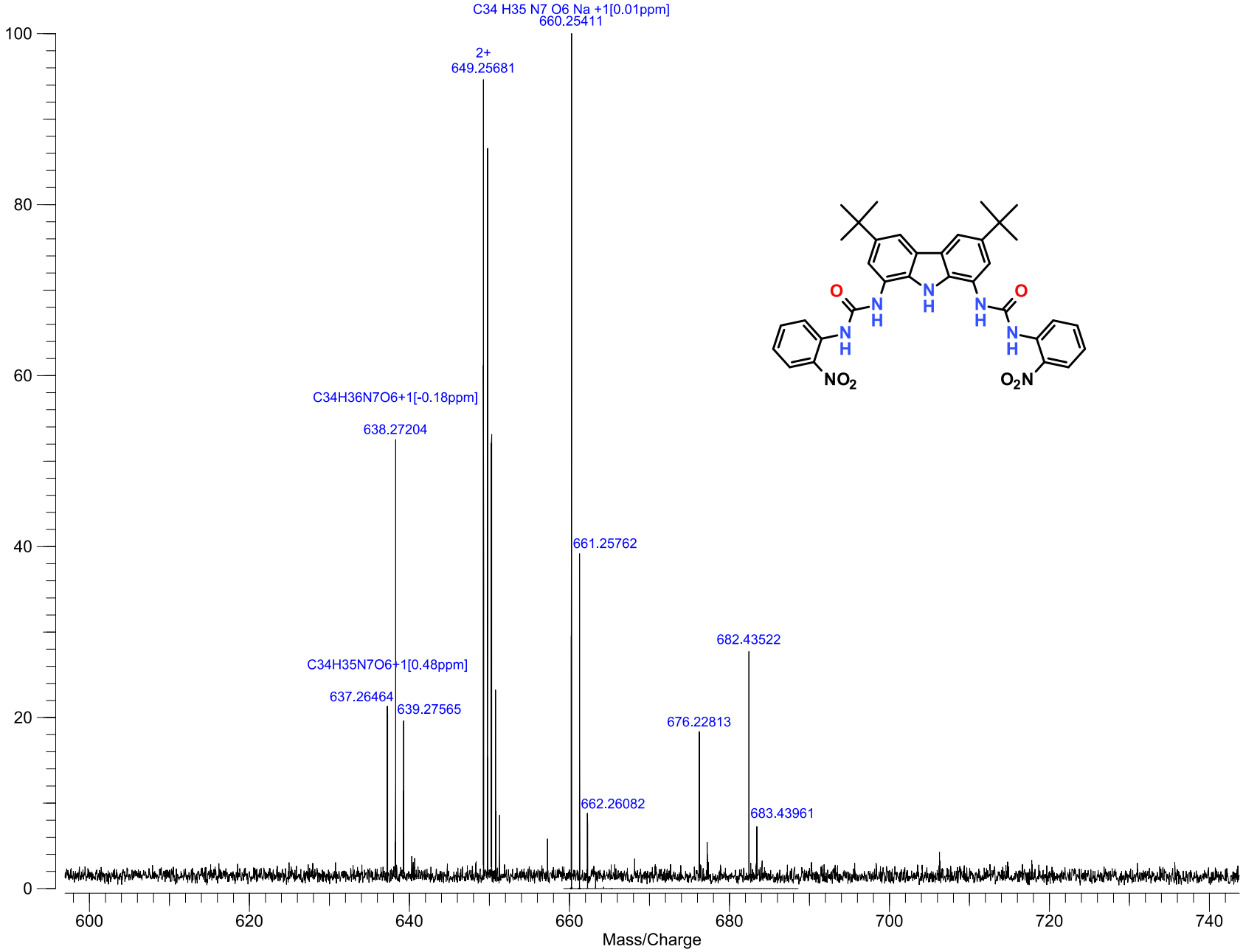
^{1}H NMR spectrum of compound CZ06



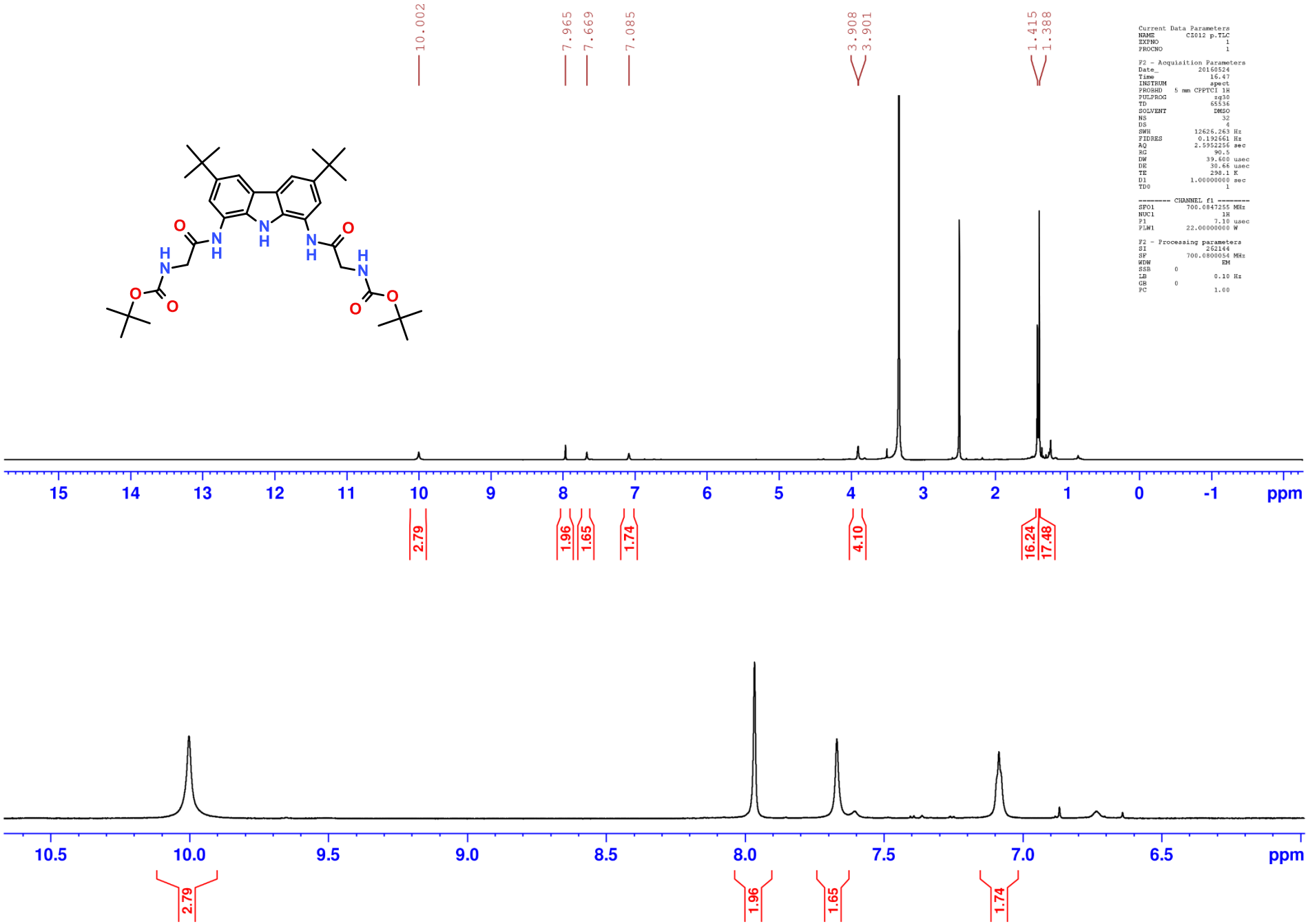
^{13}C NMR spectrum of compound CZ06



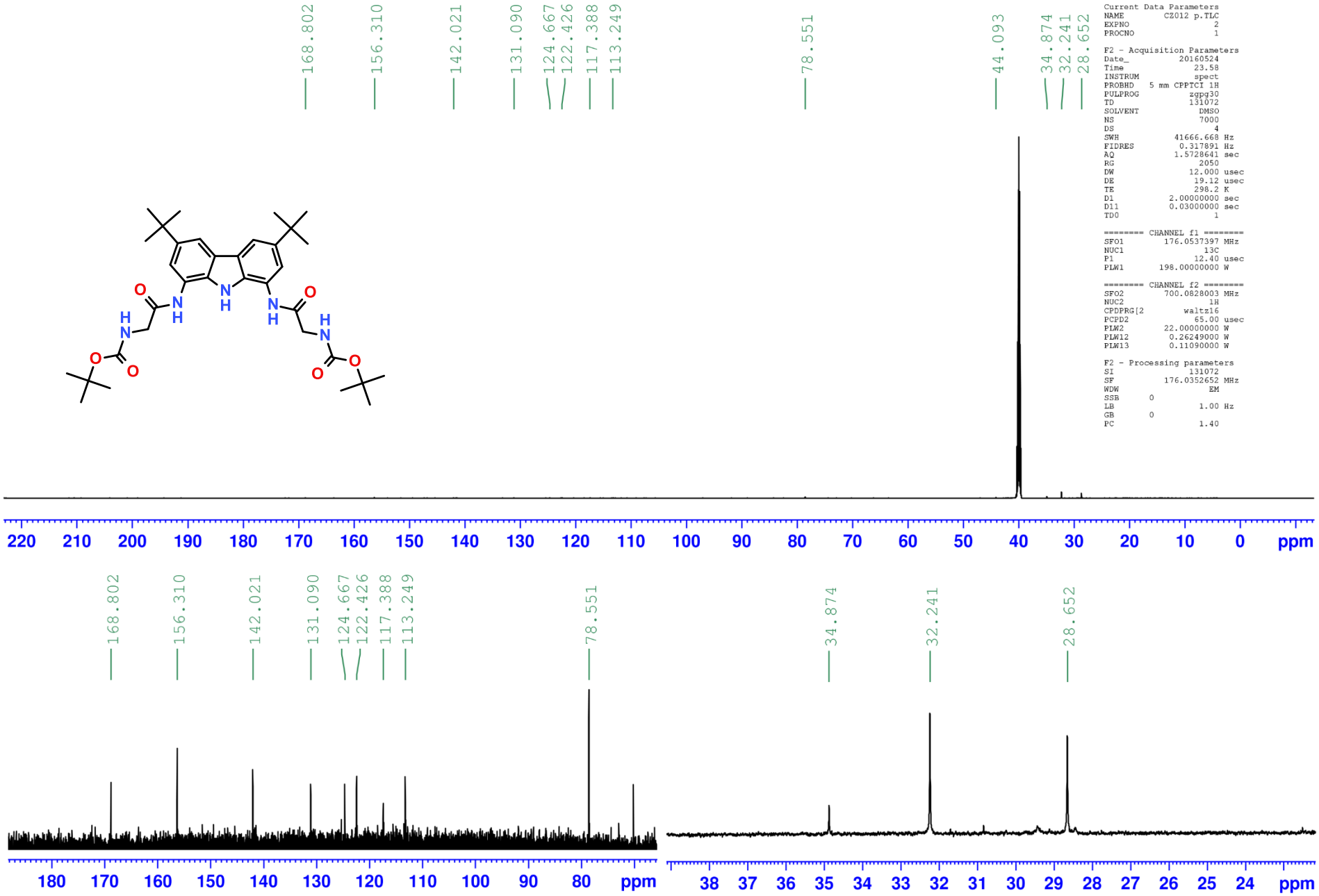
HRMS spectrum of compound CZ06



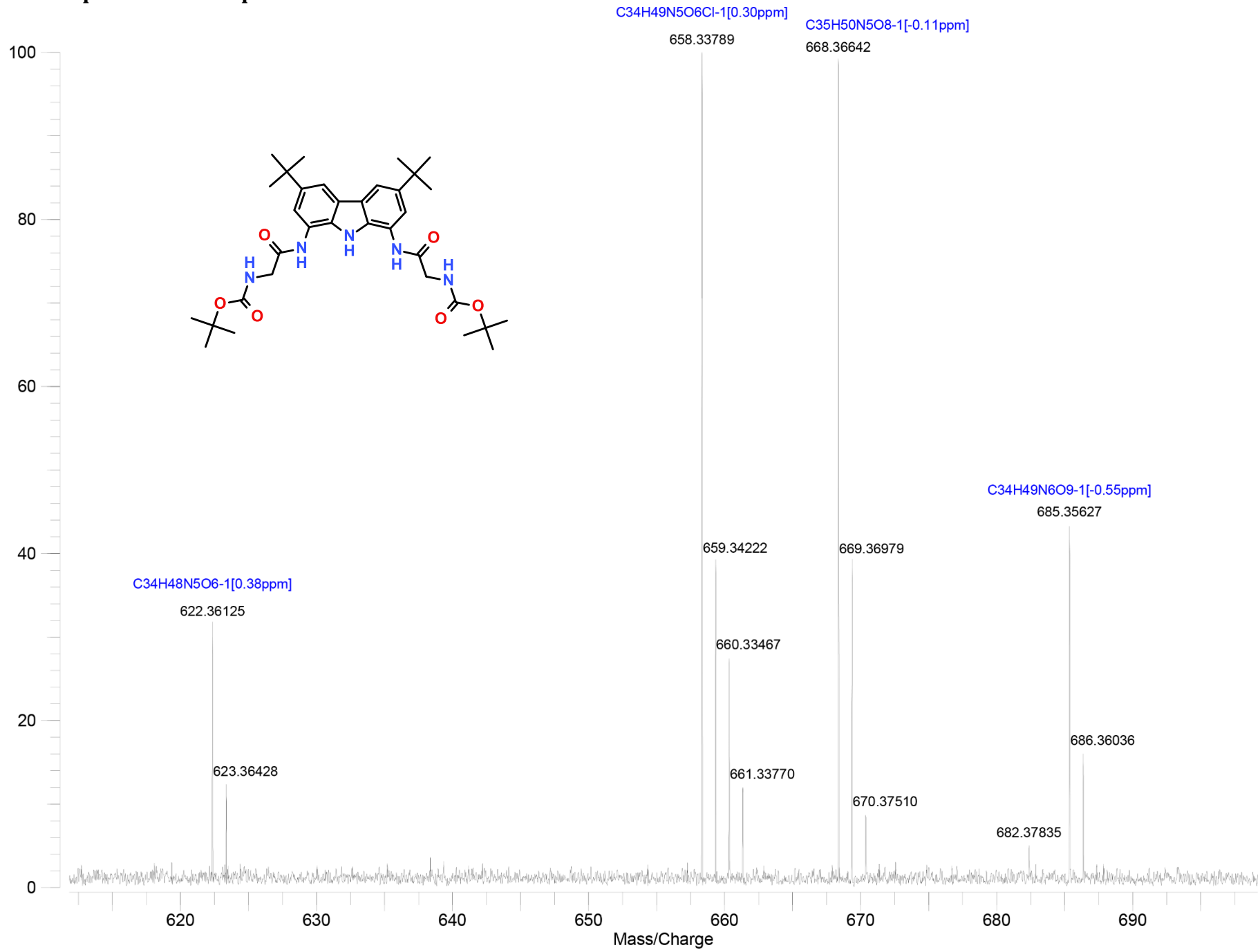
^{1}H NMR spectrum of compound CZ07



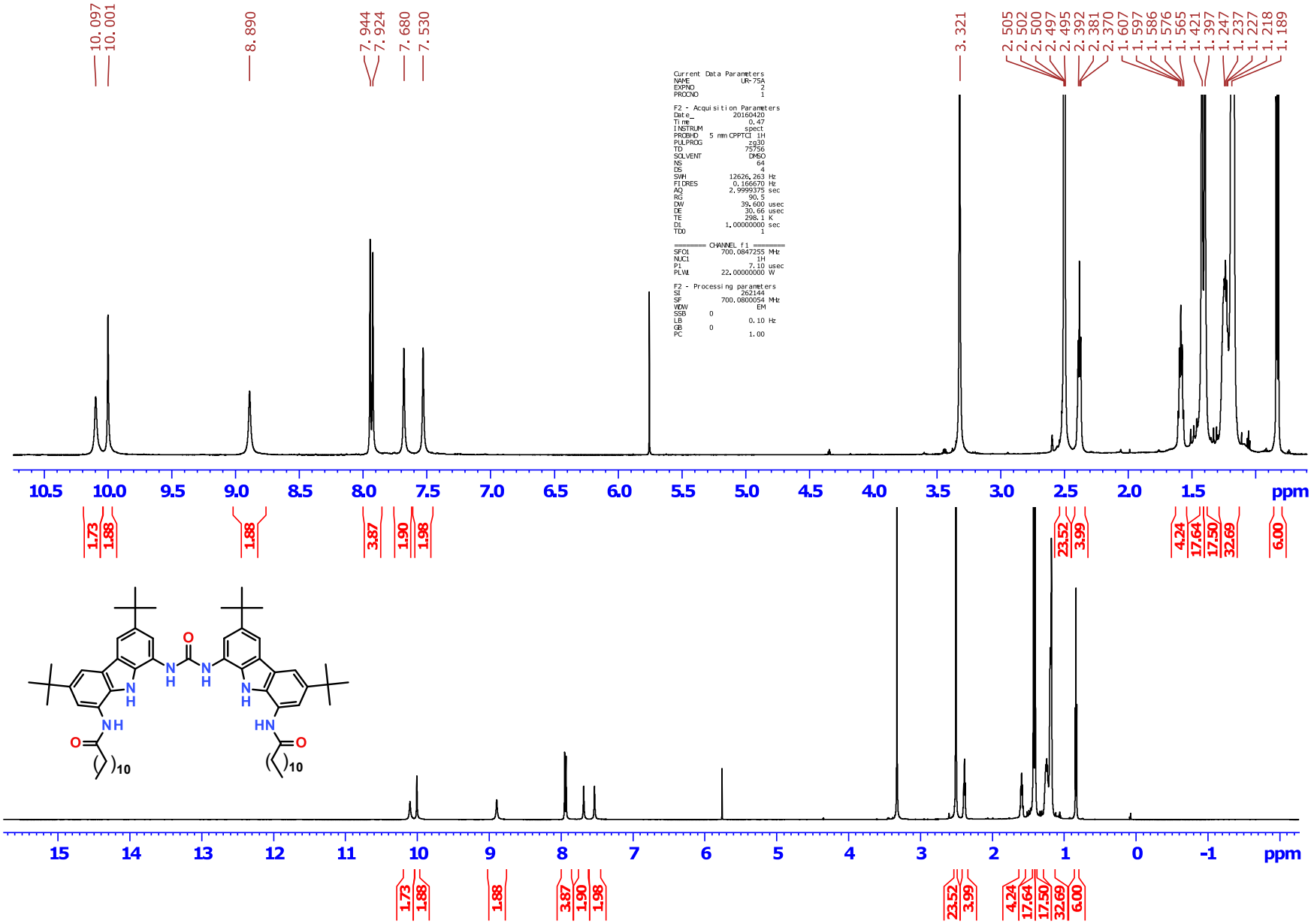
^{13}C NMR spectrum of compound CZ07



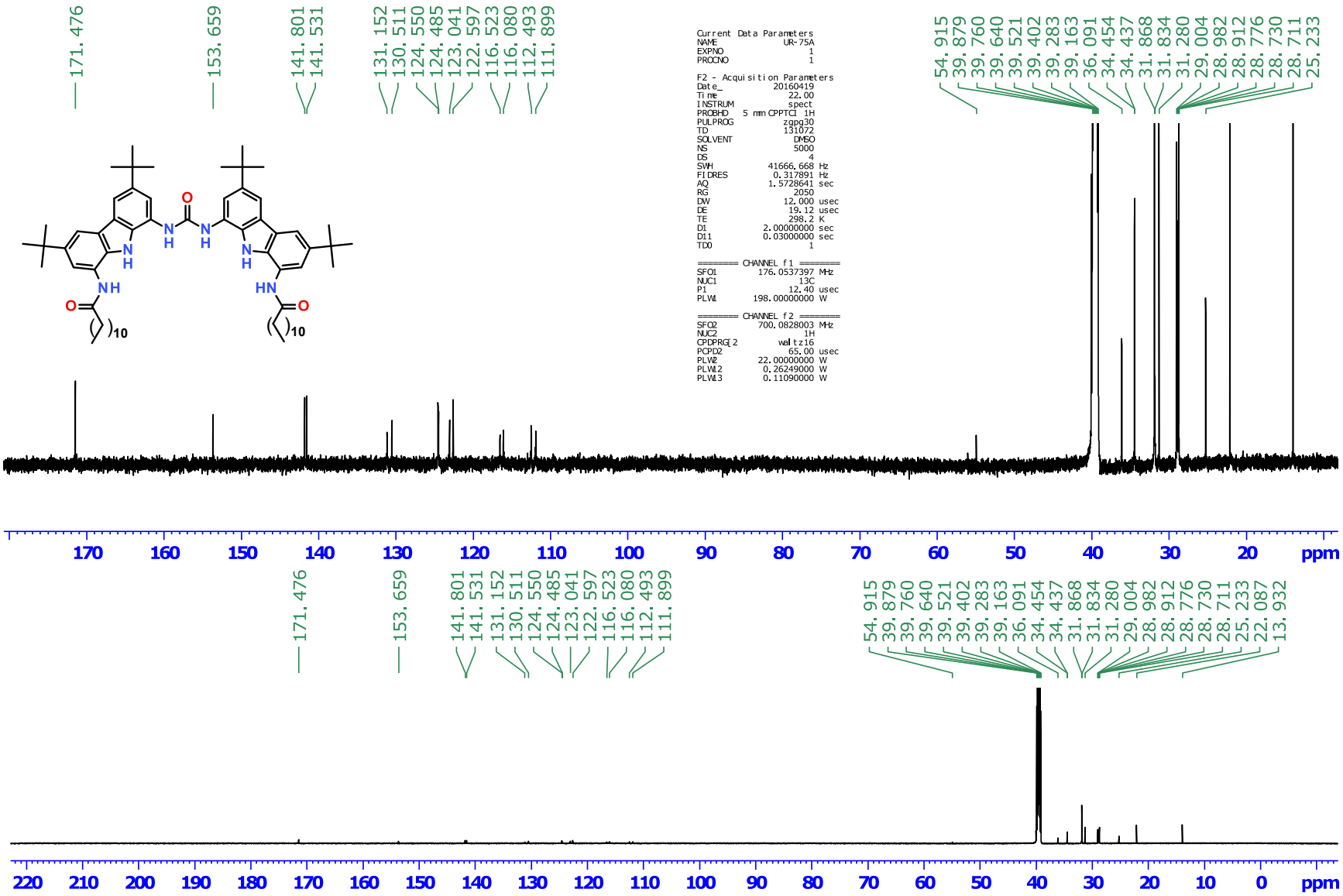
HRMS spectrum of compound CZ07



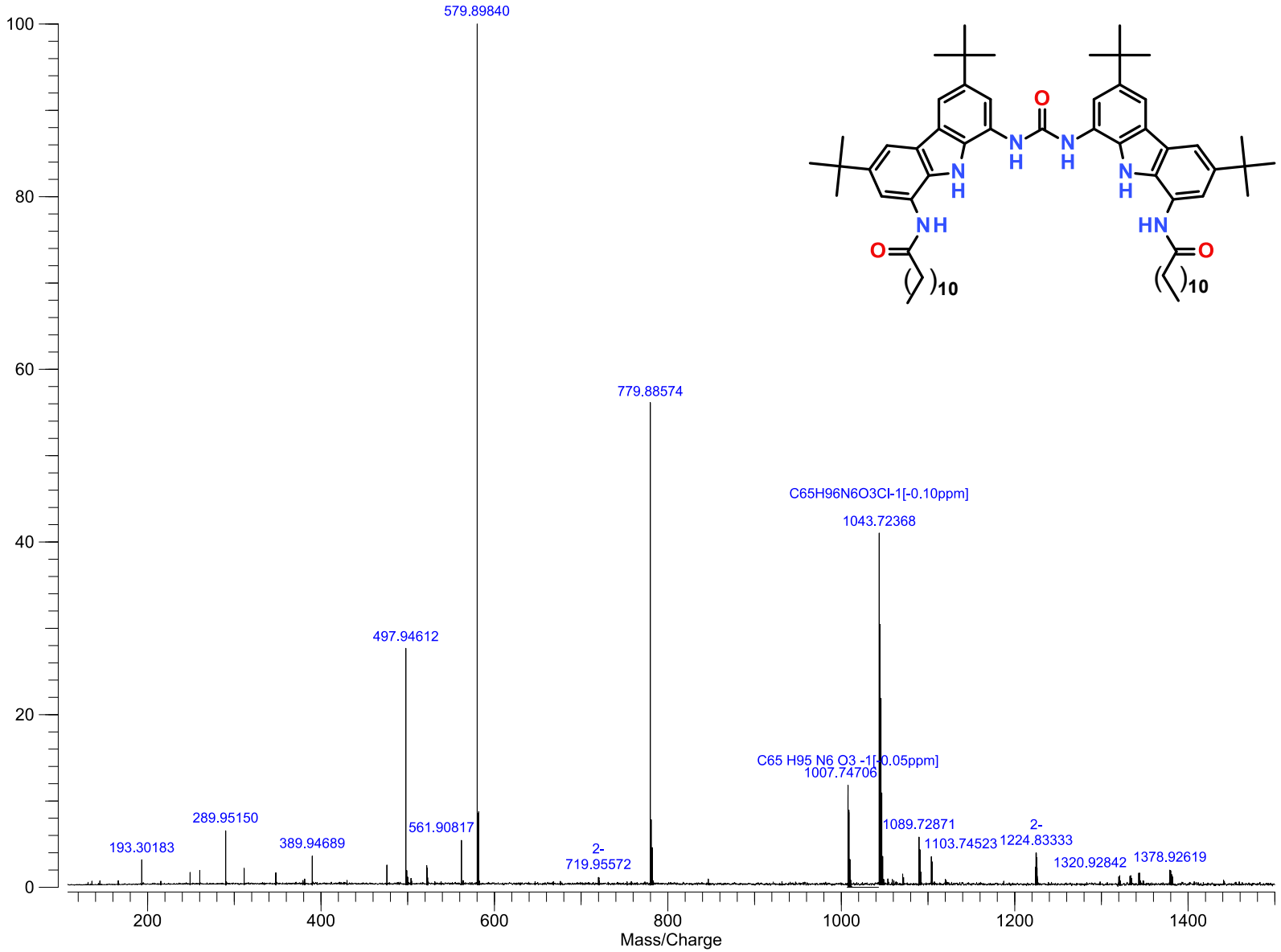
^{1}H NMR spectrum of compound CZ09



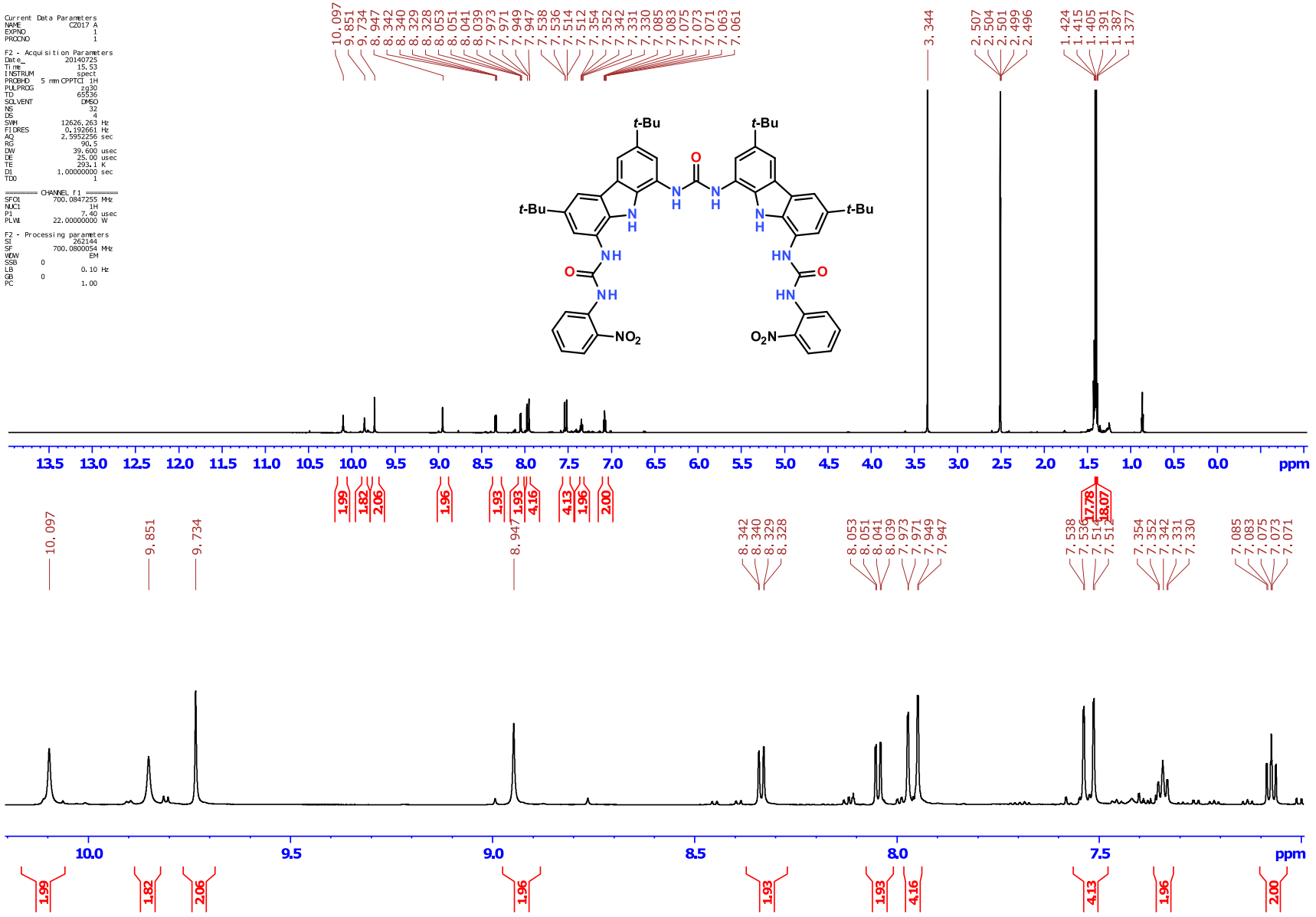
^{13}C NMR spectrum of compound CZ09



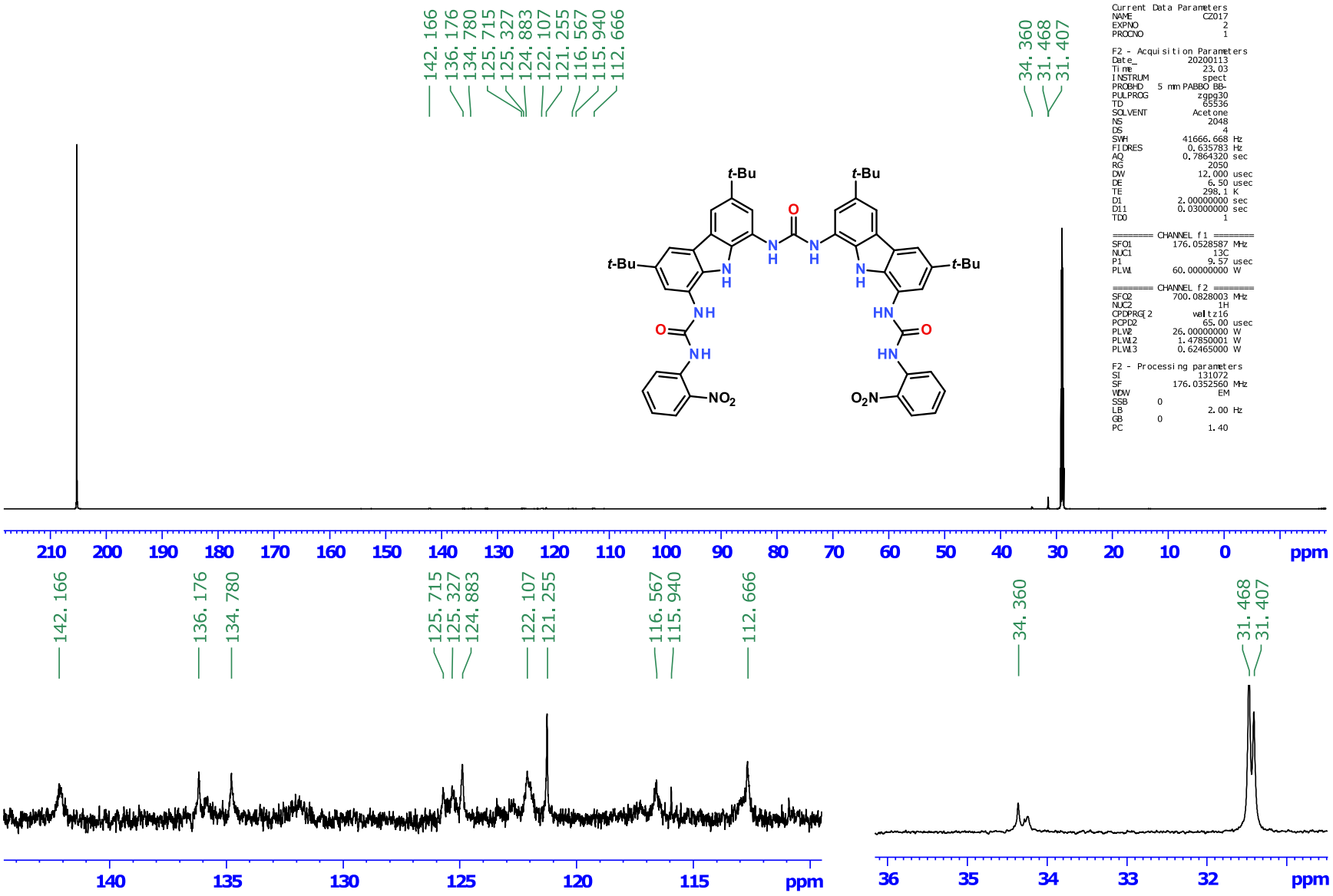
HRMS spectrum of compound CZ09



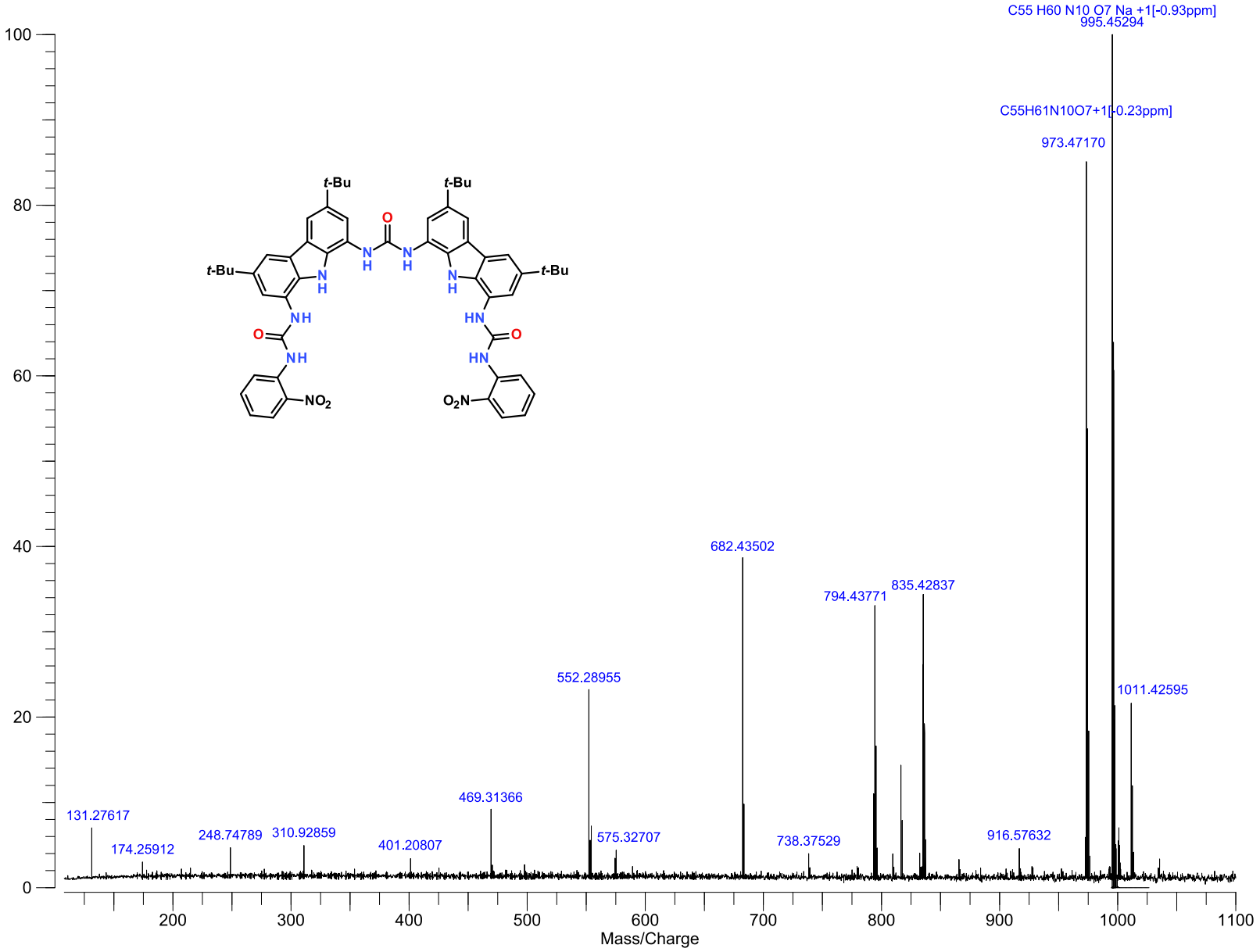
^{1}H NMR spectrum of compound CZ12



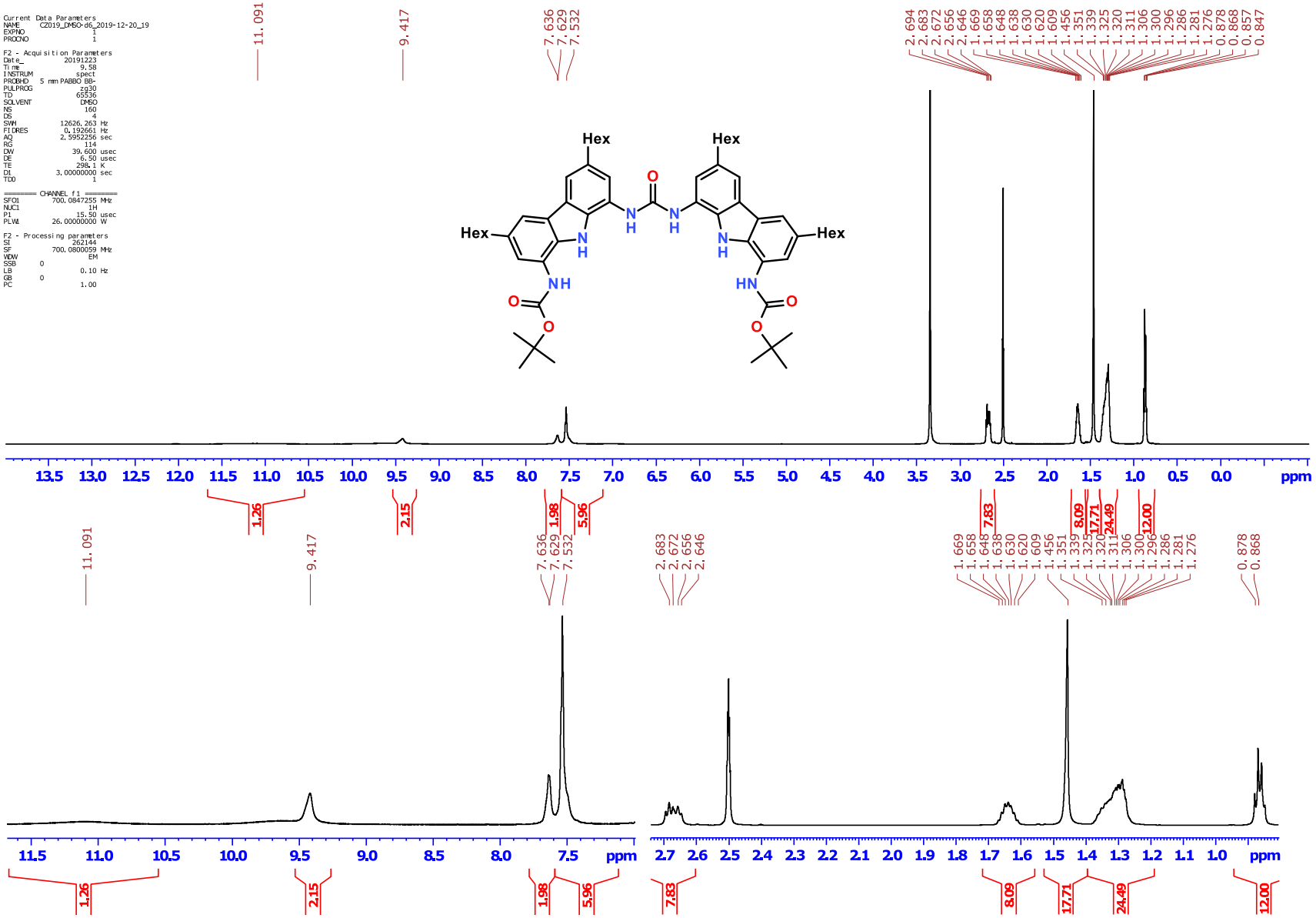
^{13}C NMR spectrum of compound CZ12



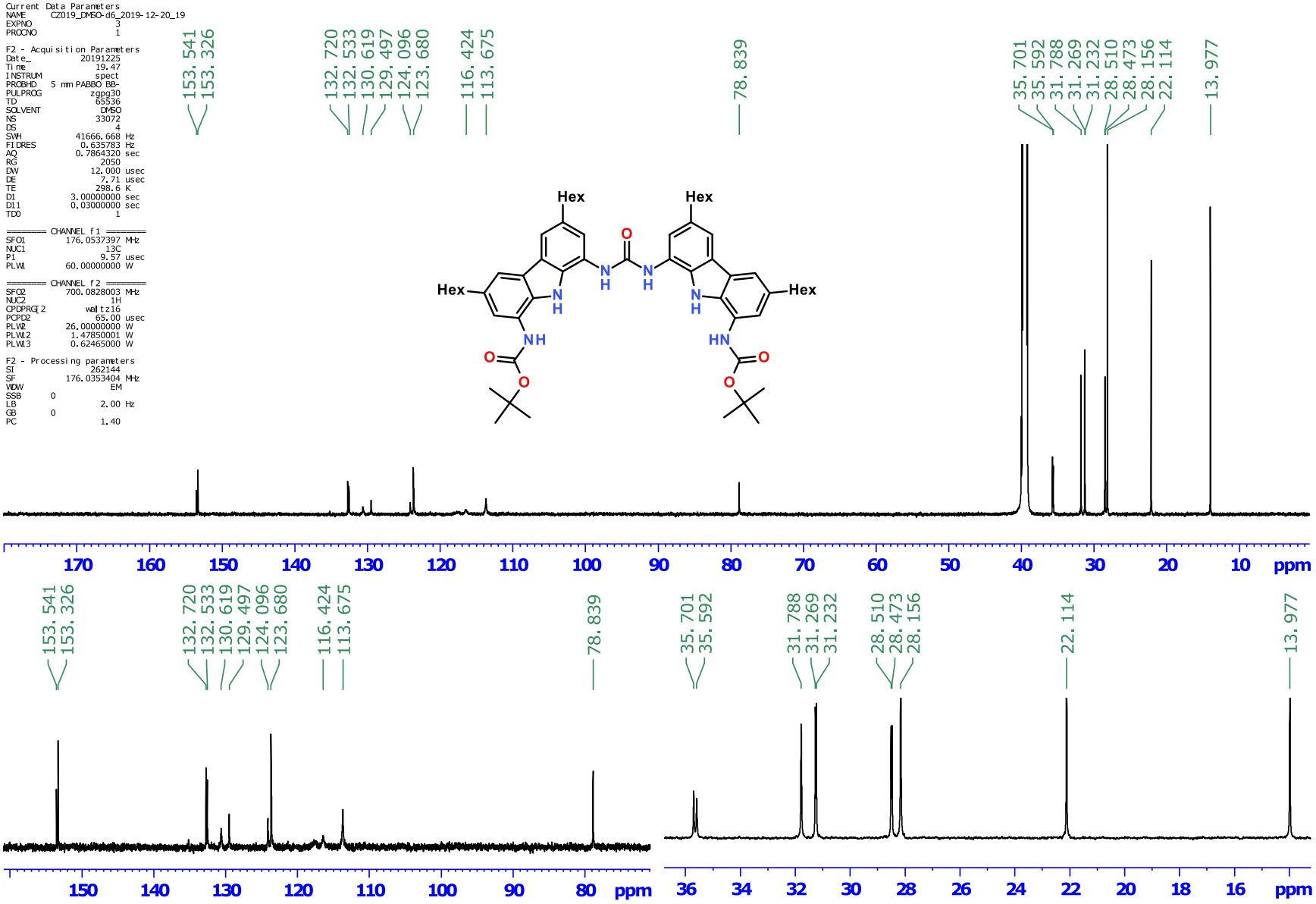
HRMS spectrum of compound CZ12



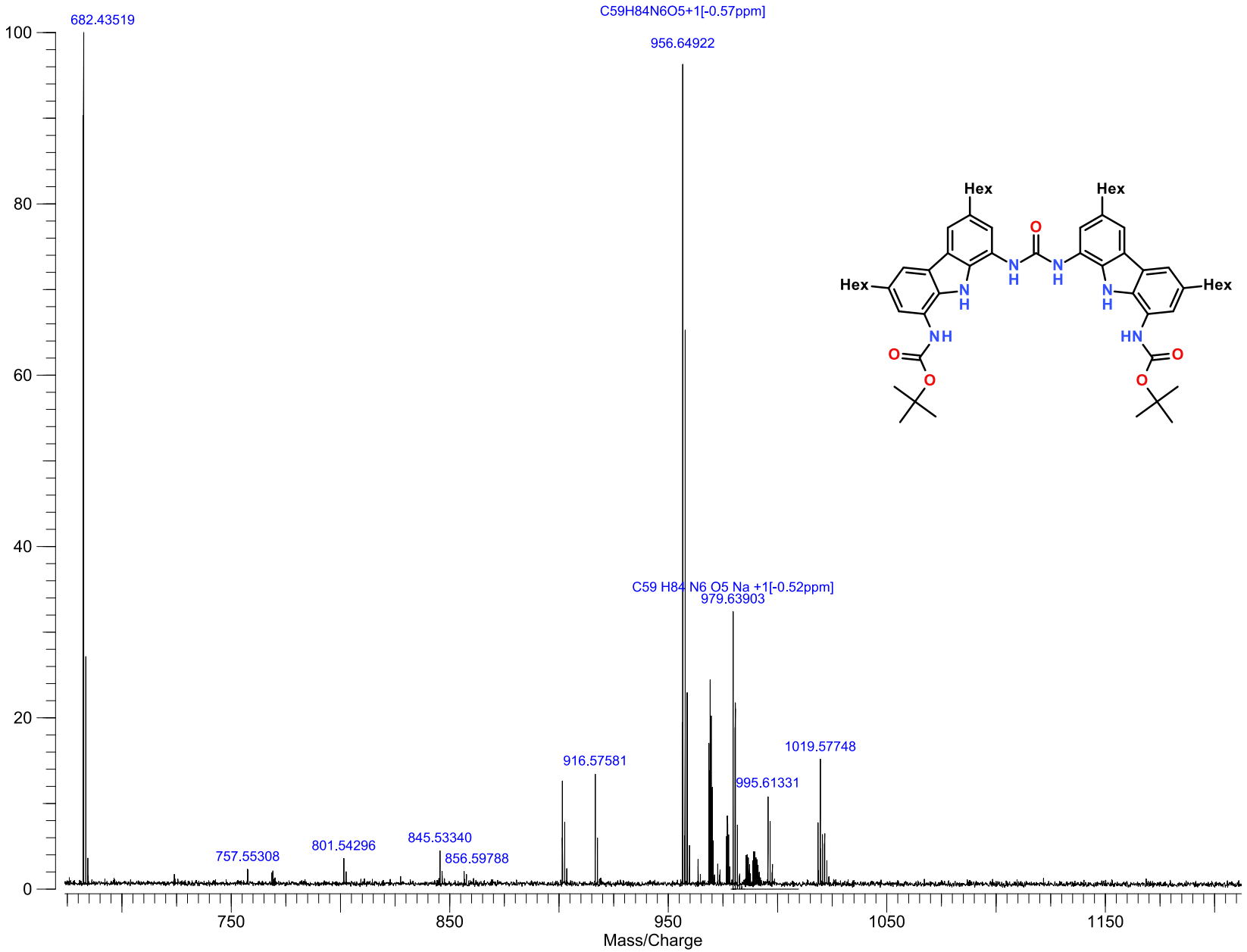
^{1}H NMR spectrum of compound CZ13



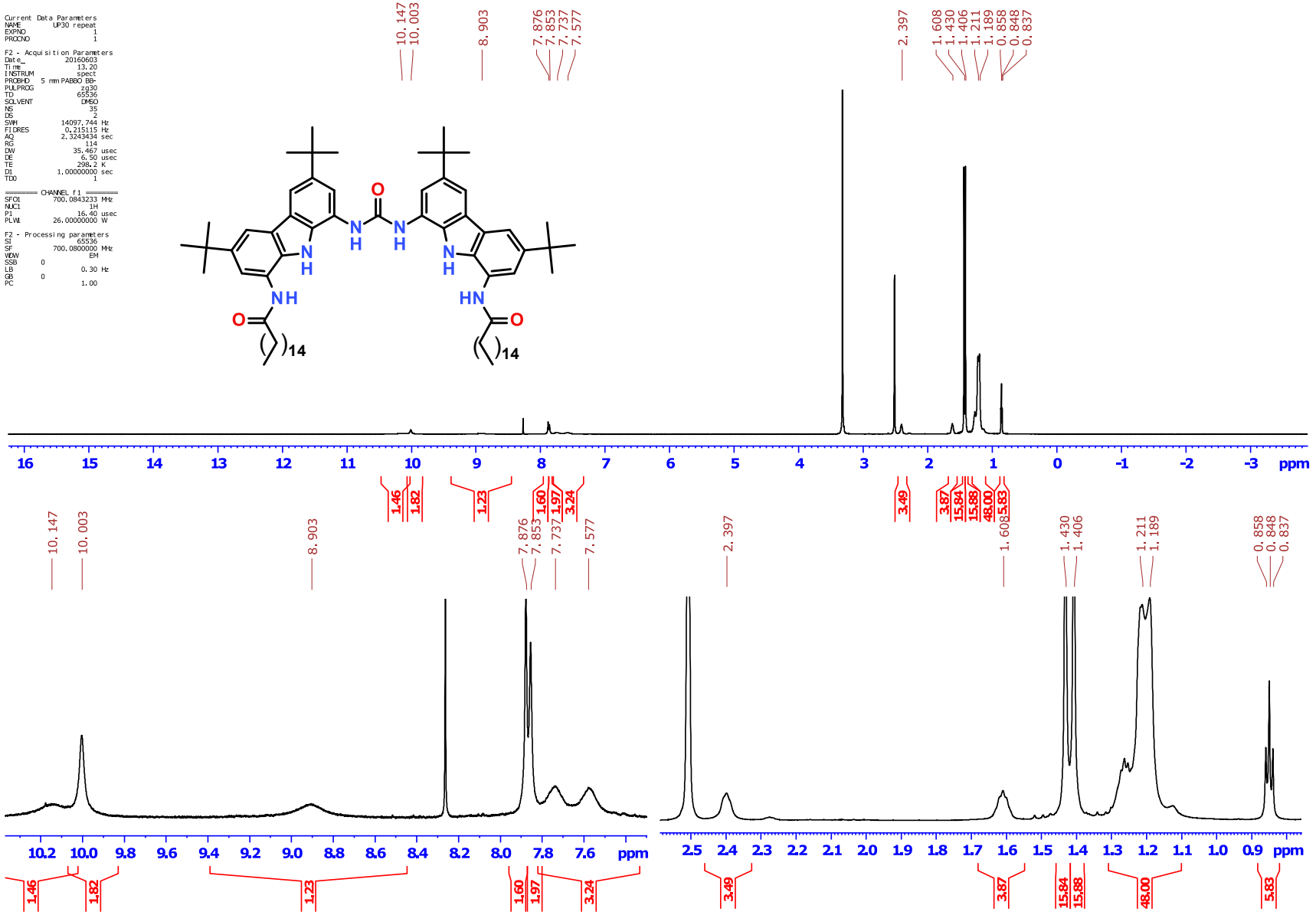
^{13}C NMR spectrum of compound CZ13



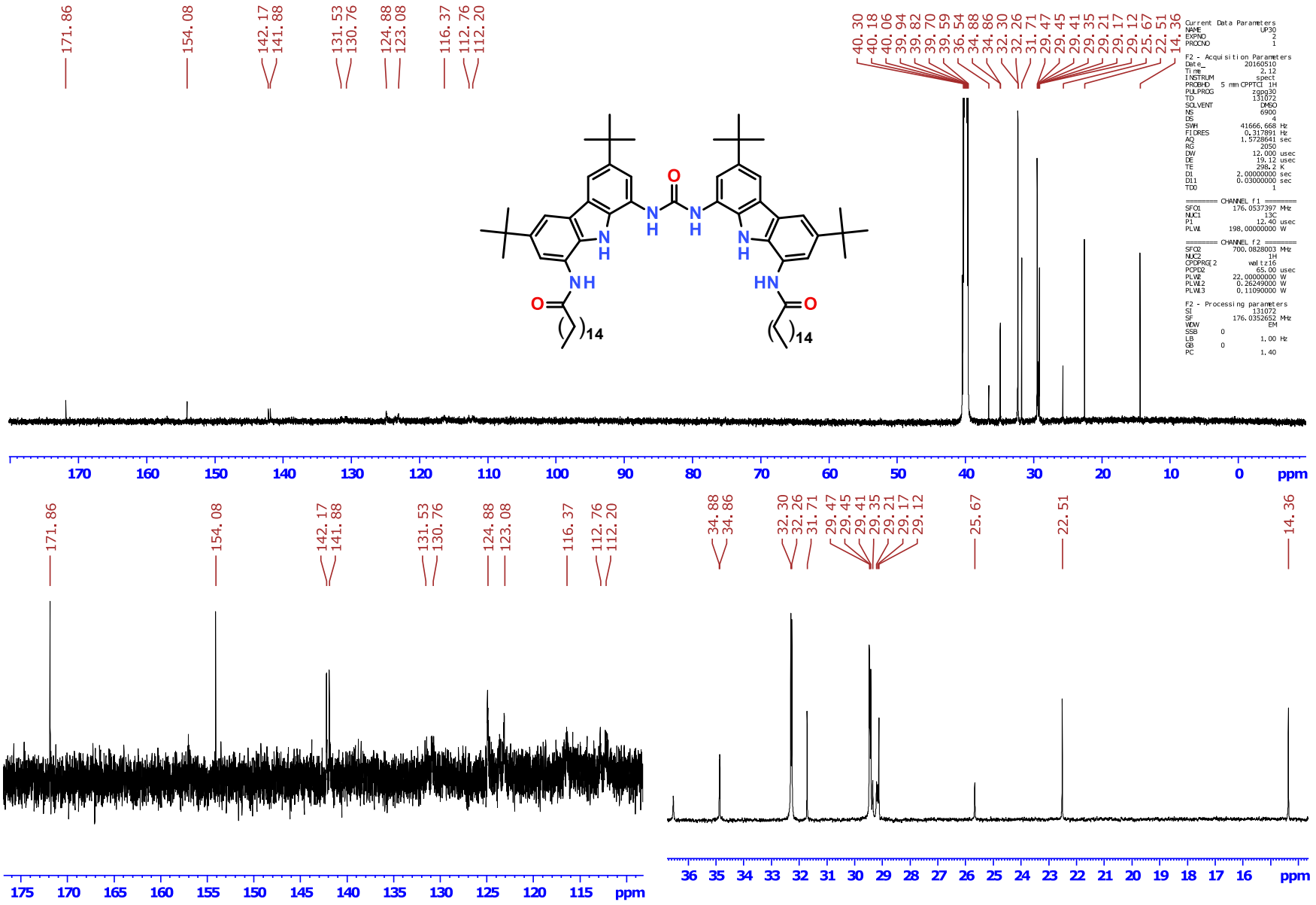
HRMS spectrum of compound CZ13



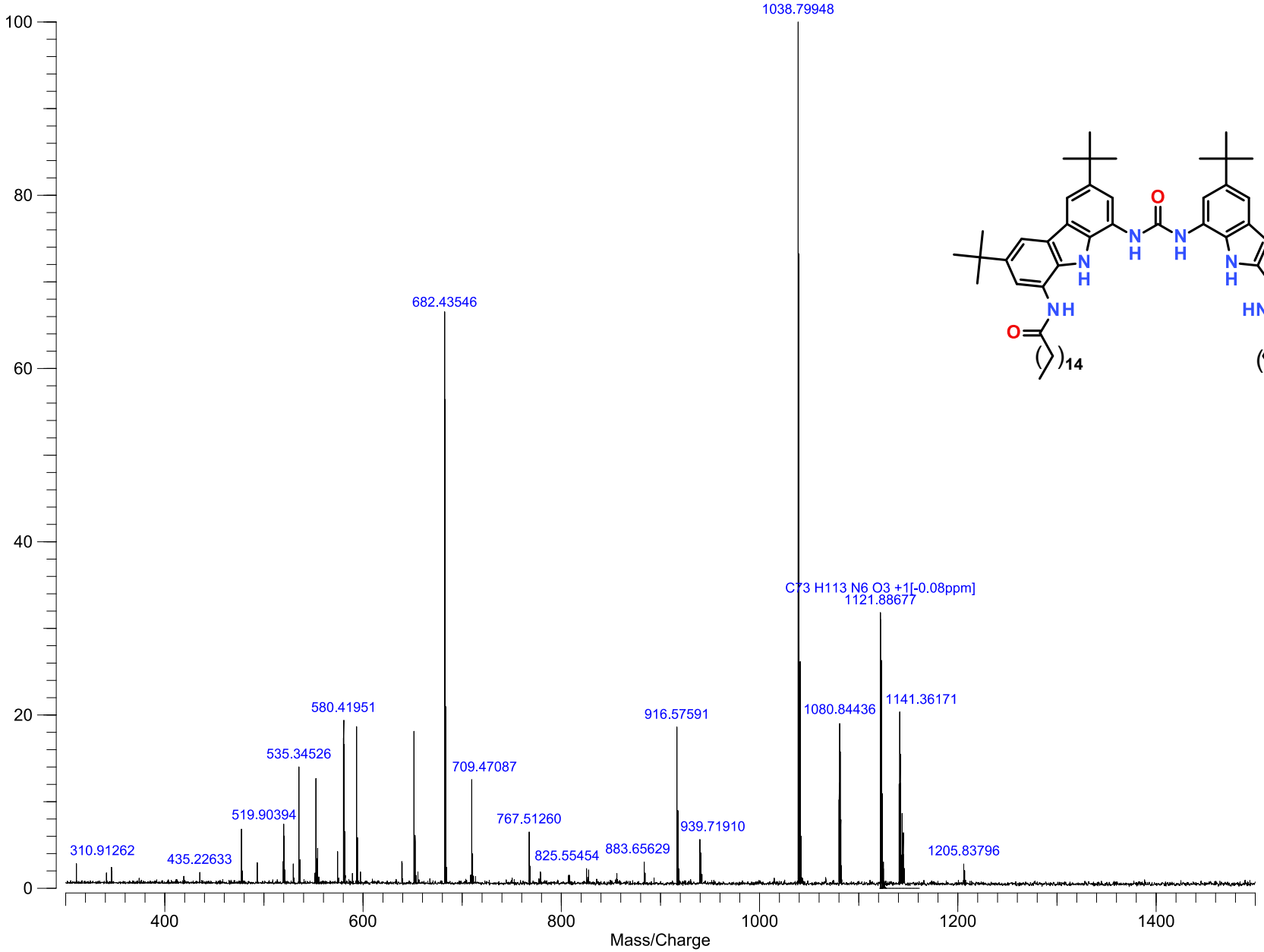
^{1}H NMR spectrum of compound CZ14



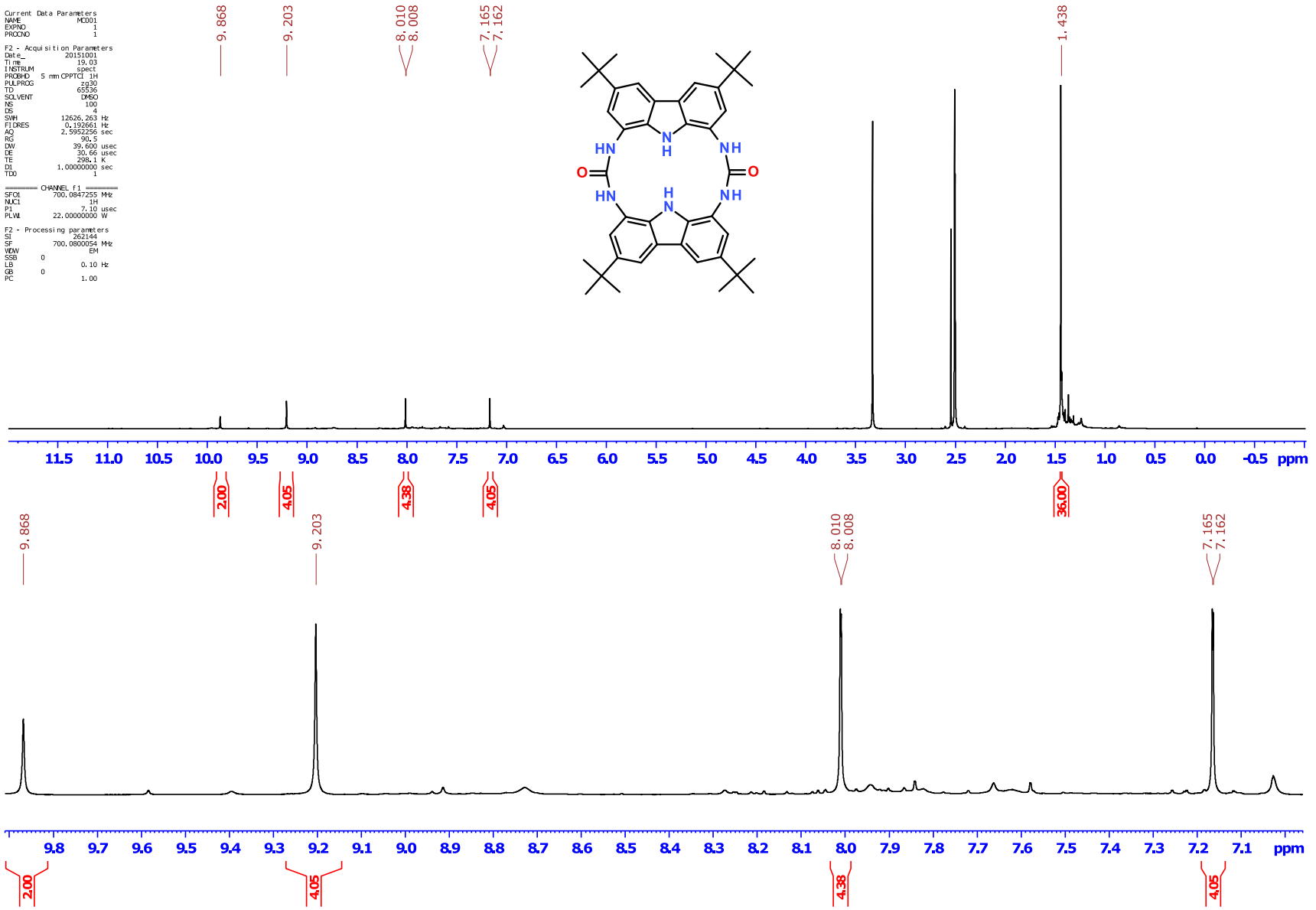
^{13}C NMR spectrum of compound CZ14



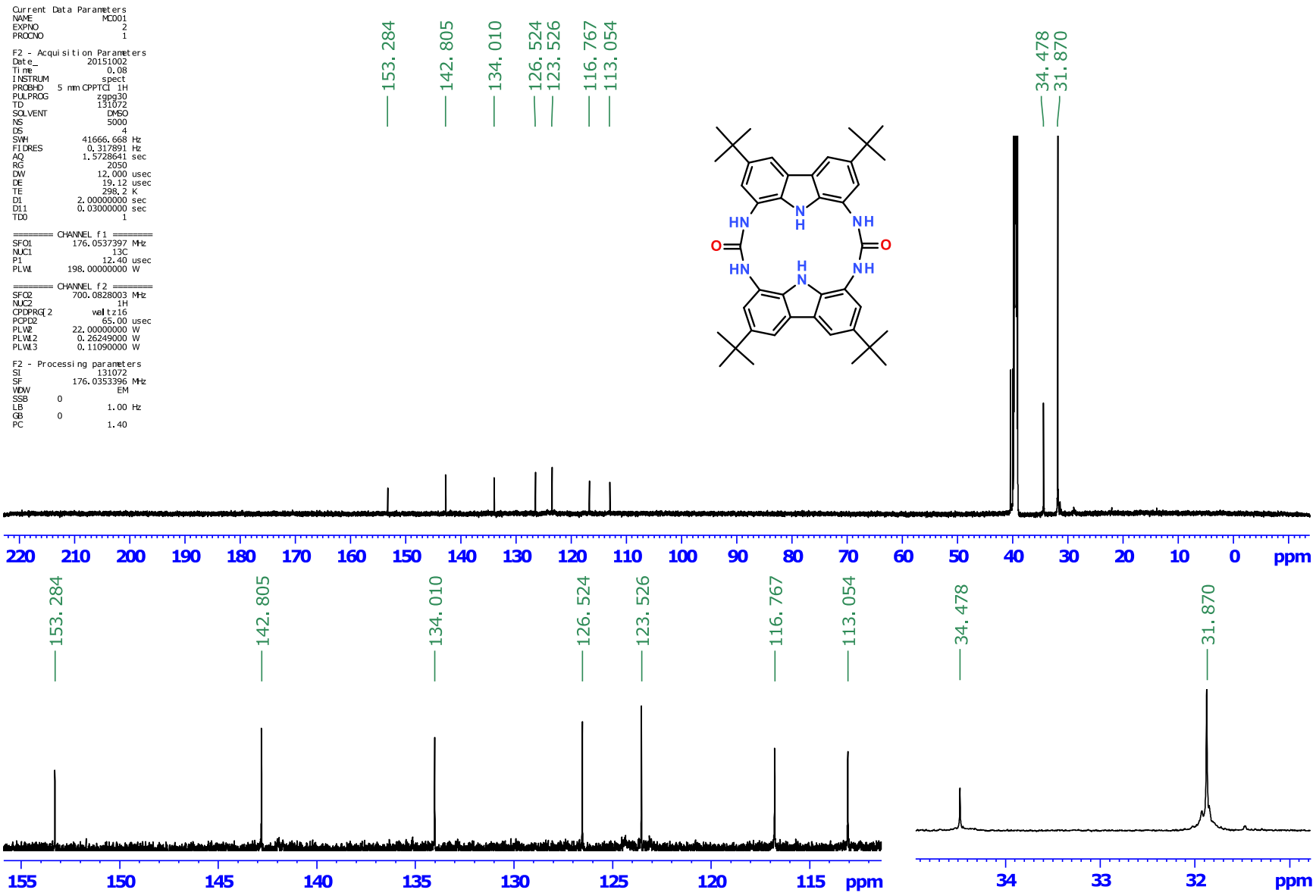
HRMS spectrum of compound CZ14



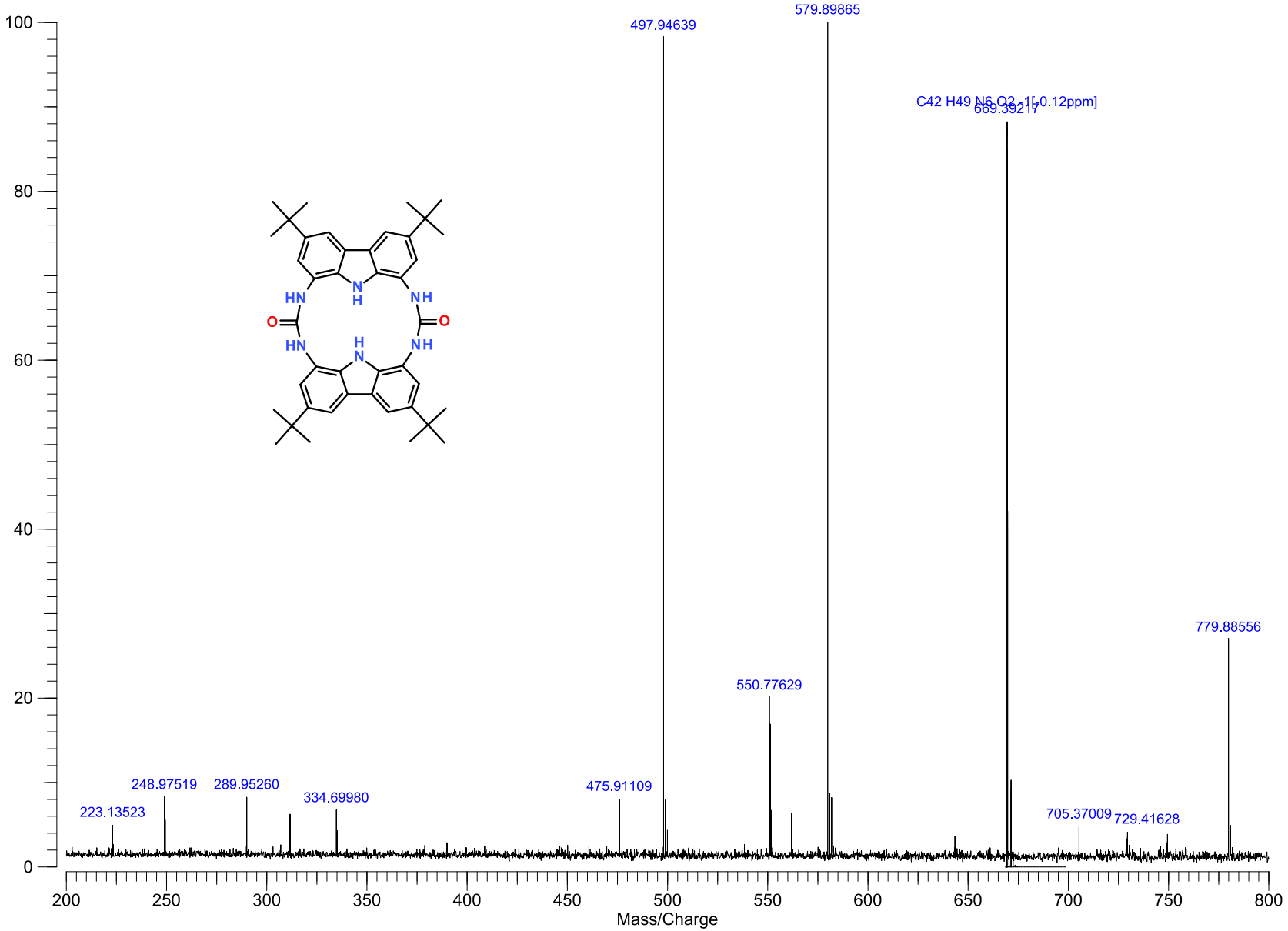
^{1}H NMR spectrum of compound MC01



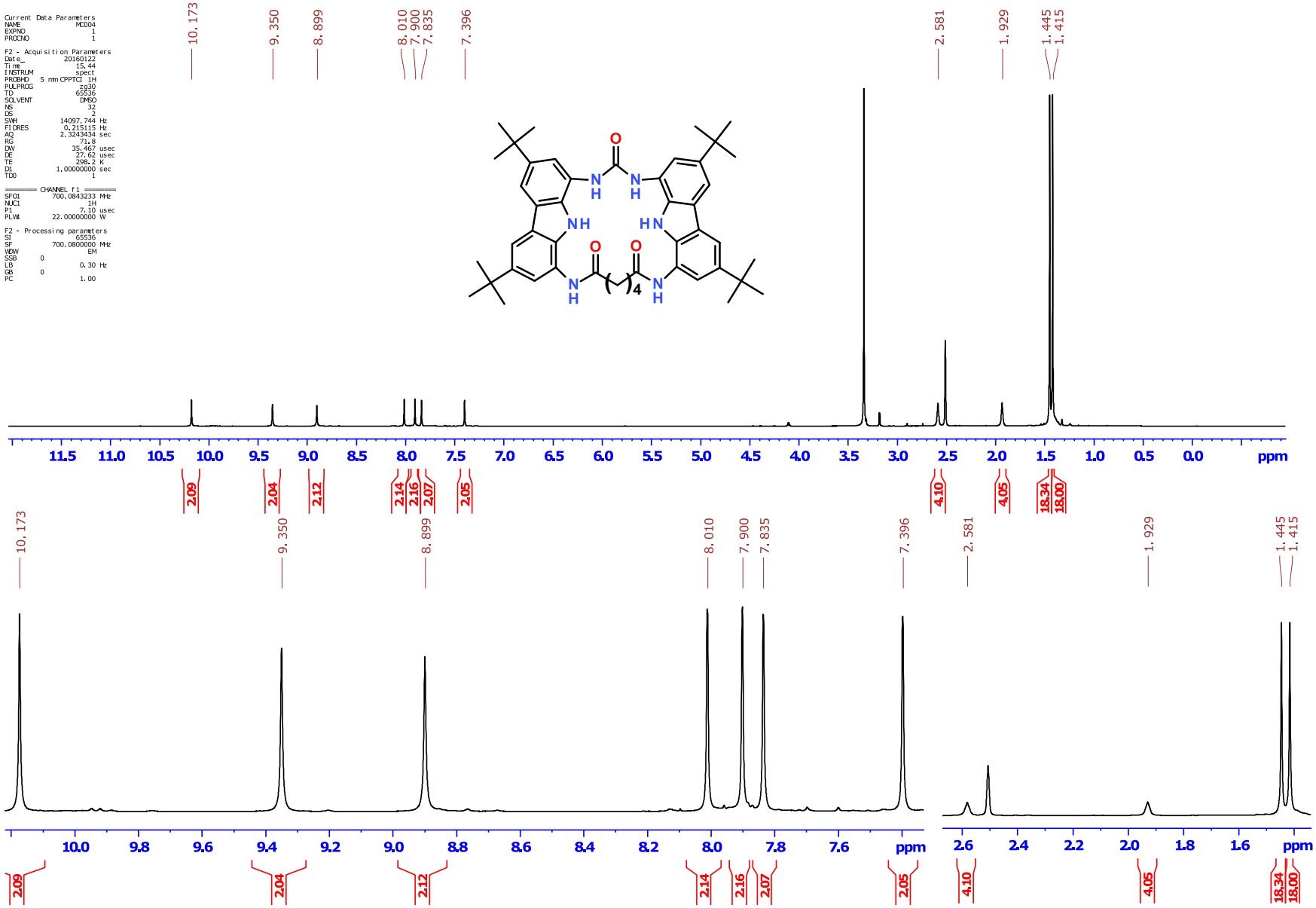
^{13}C NMR spectrum of compound MC01



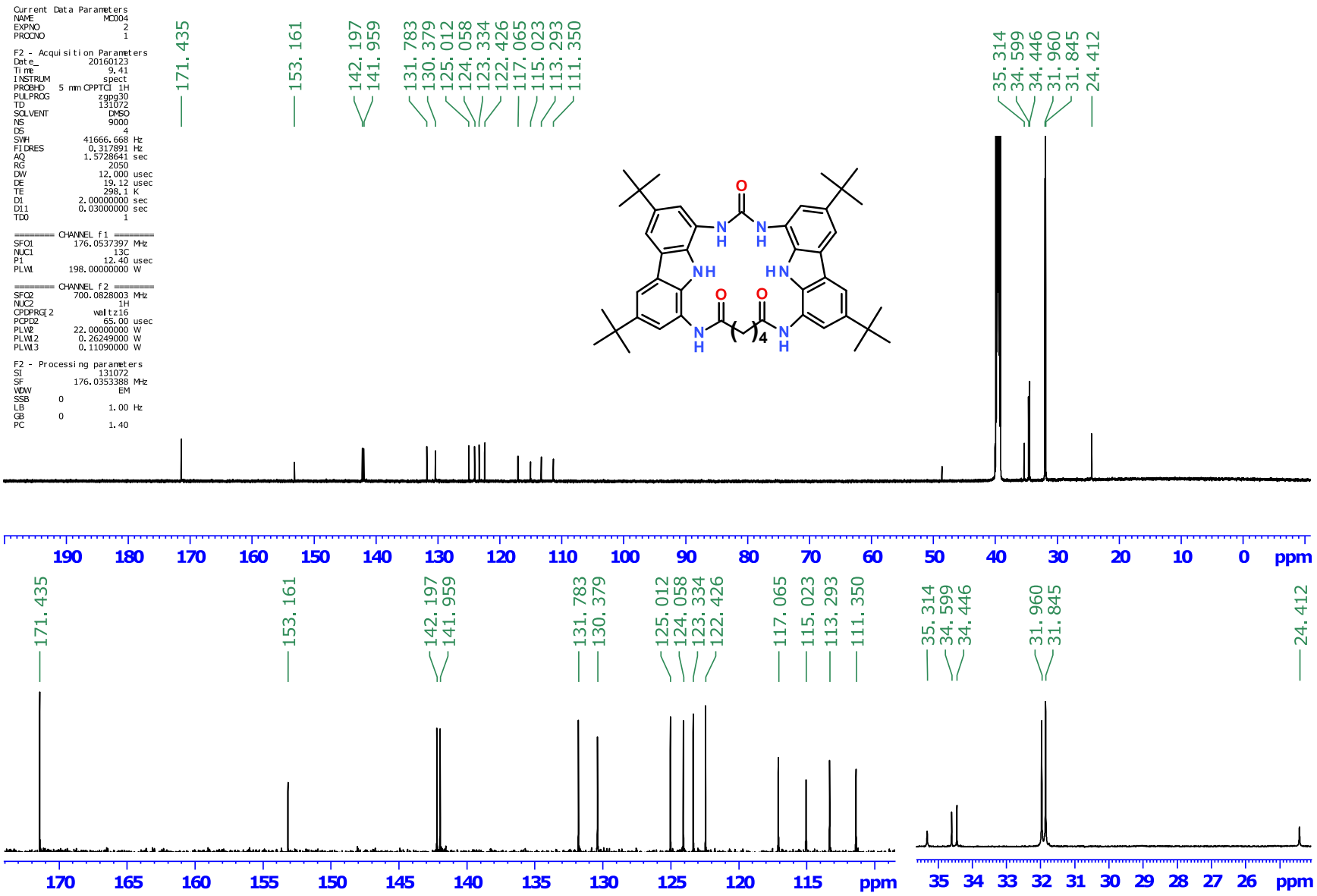
HRMS spectrum of compound MC01



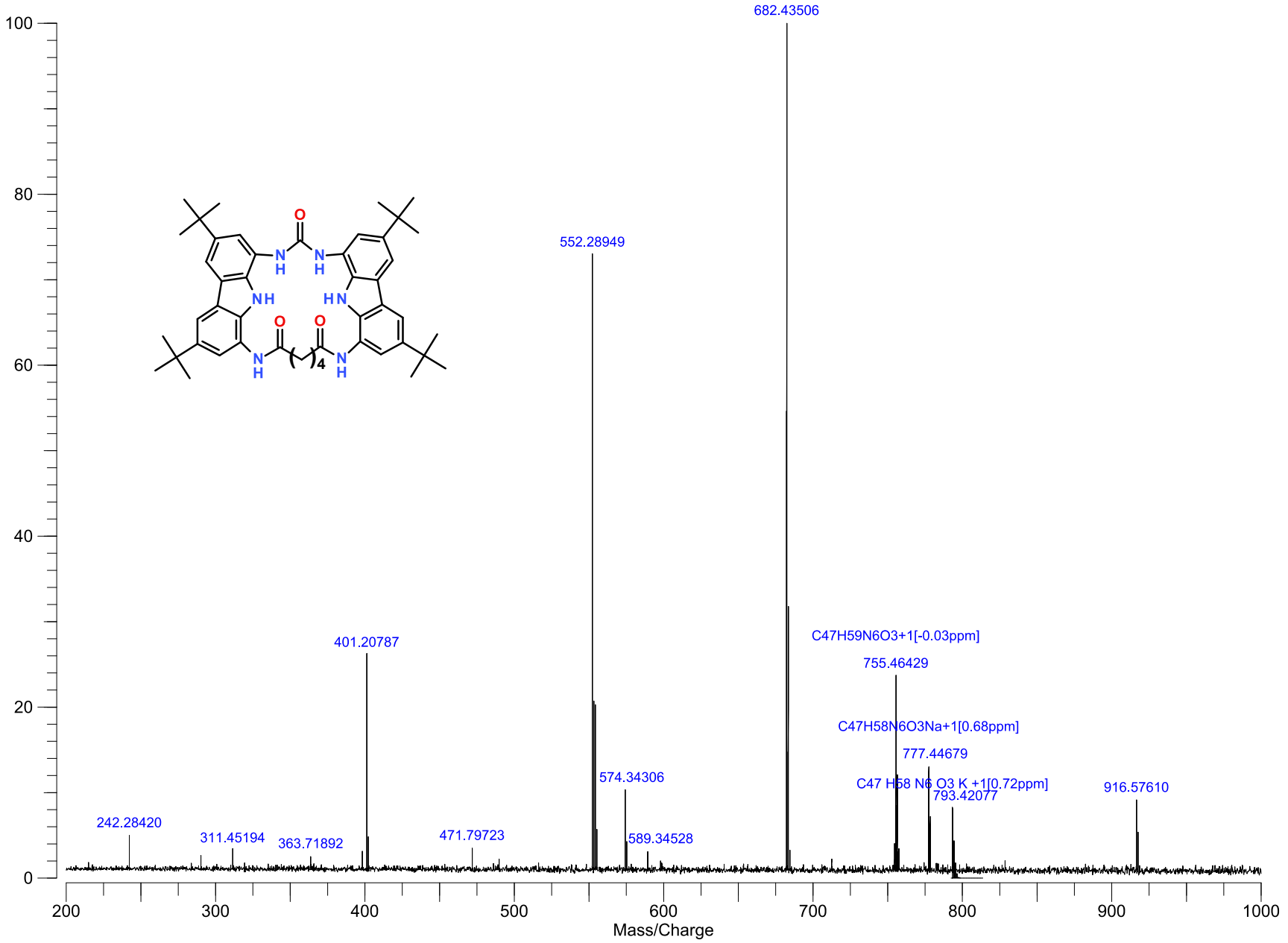
^{1}H NMR spectrum of compound MC04



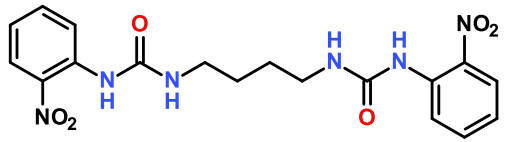
^{13}C NMR spectrum of compound MC04

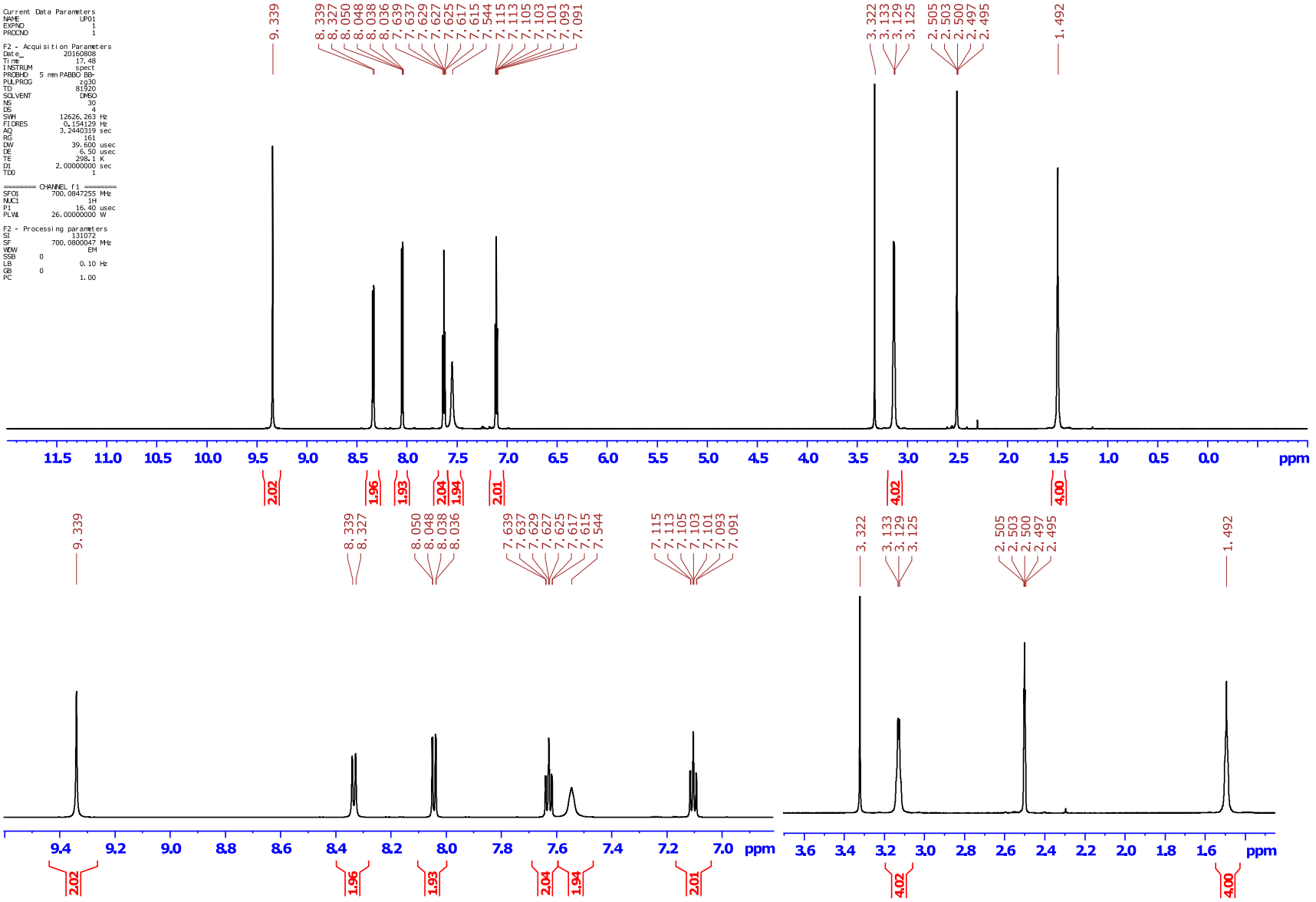


HRMS spectrum of compound MC04

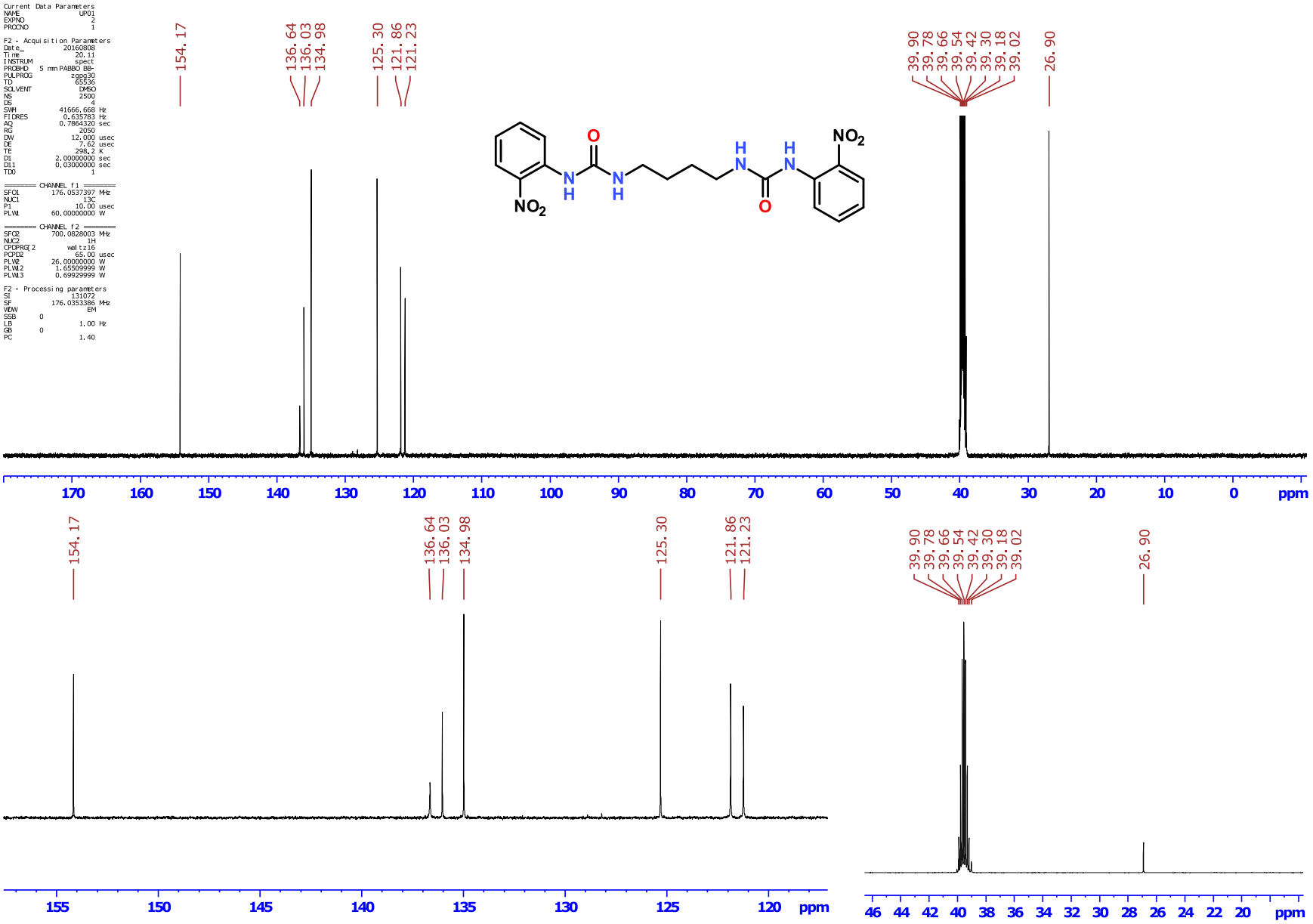


^{1}H NMR spectrum of compound U01

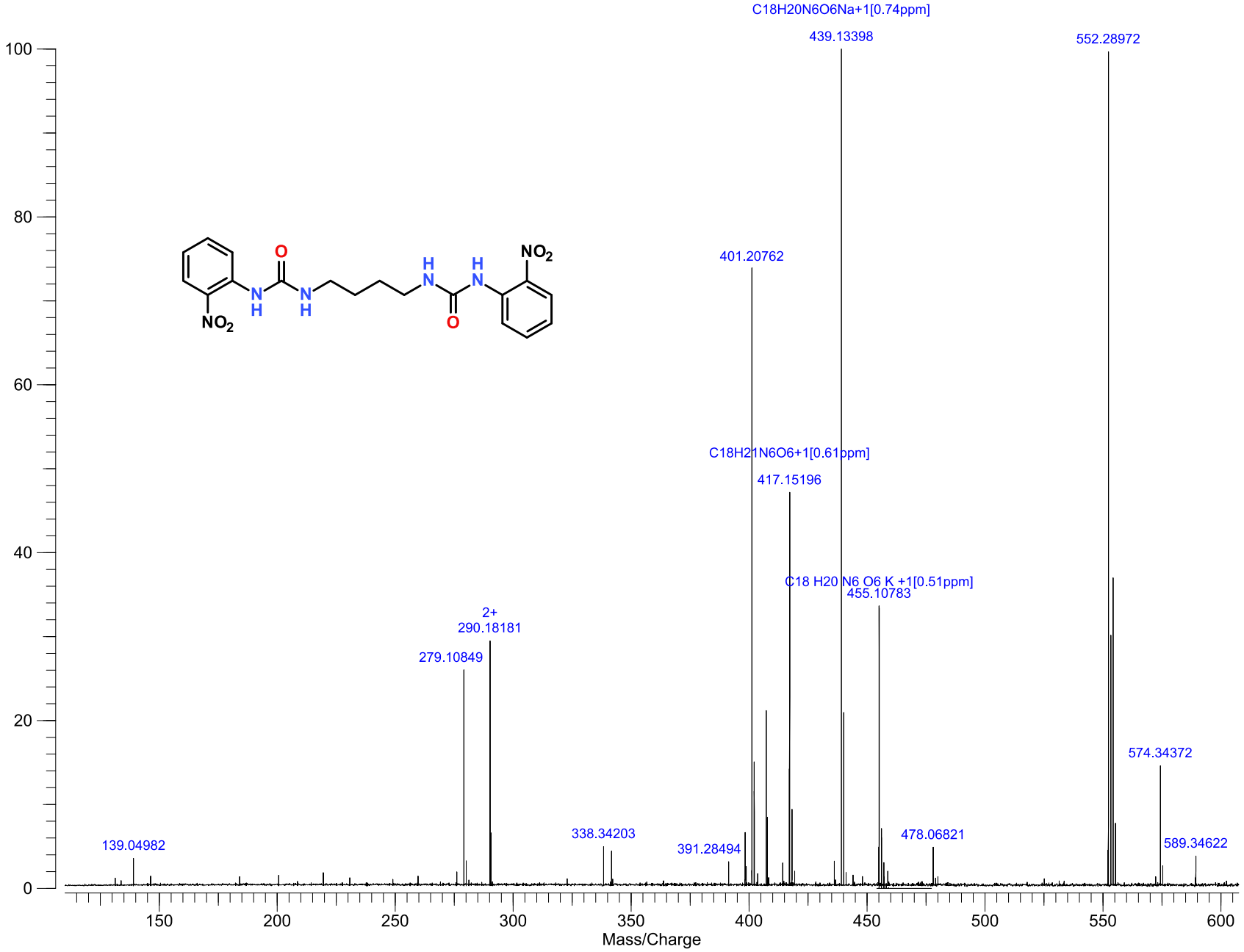




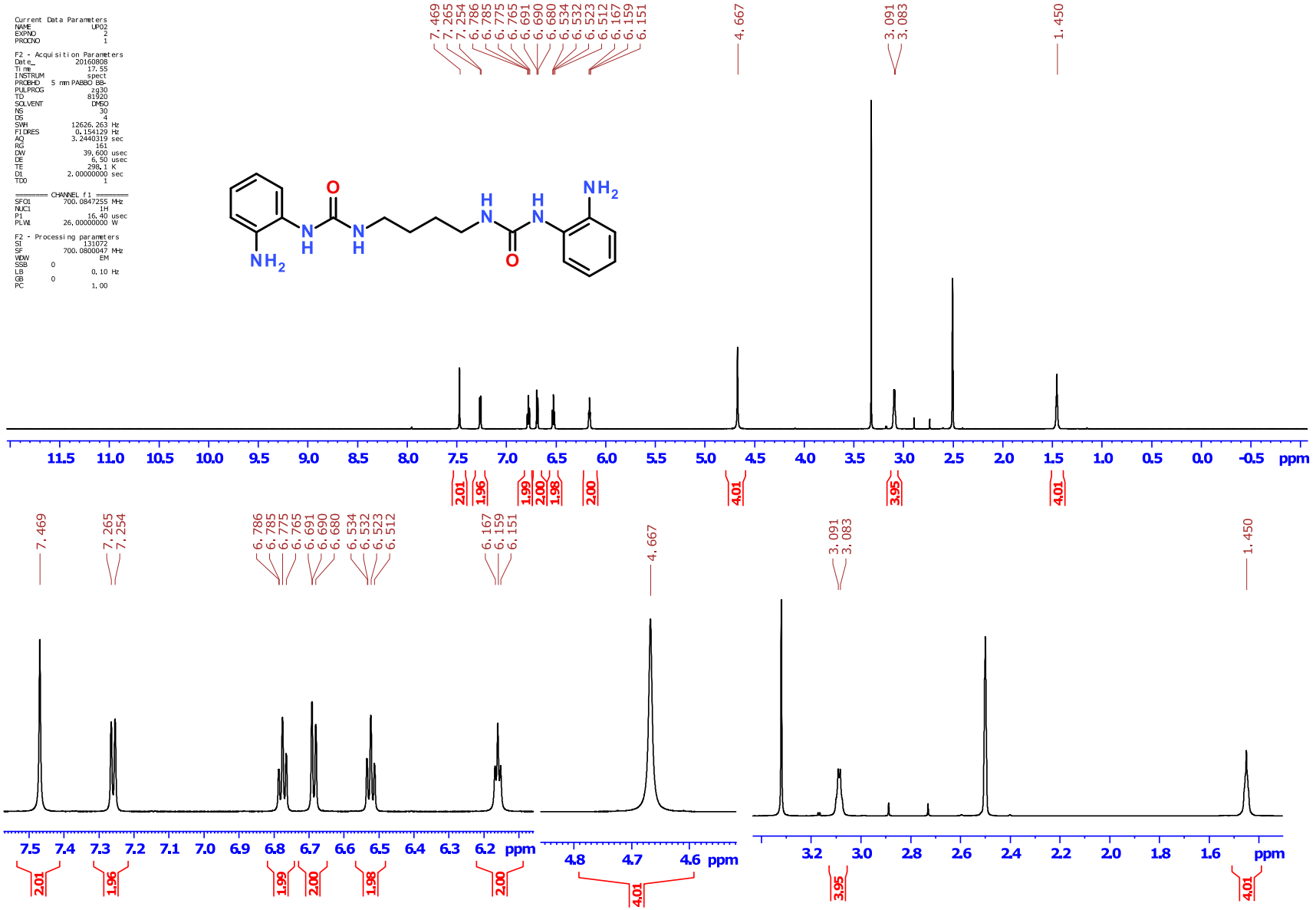
^{13}C NMR spectrum of compound U01



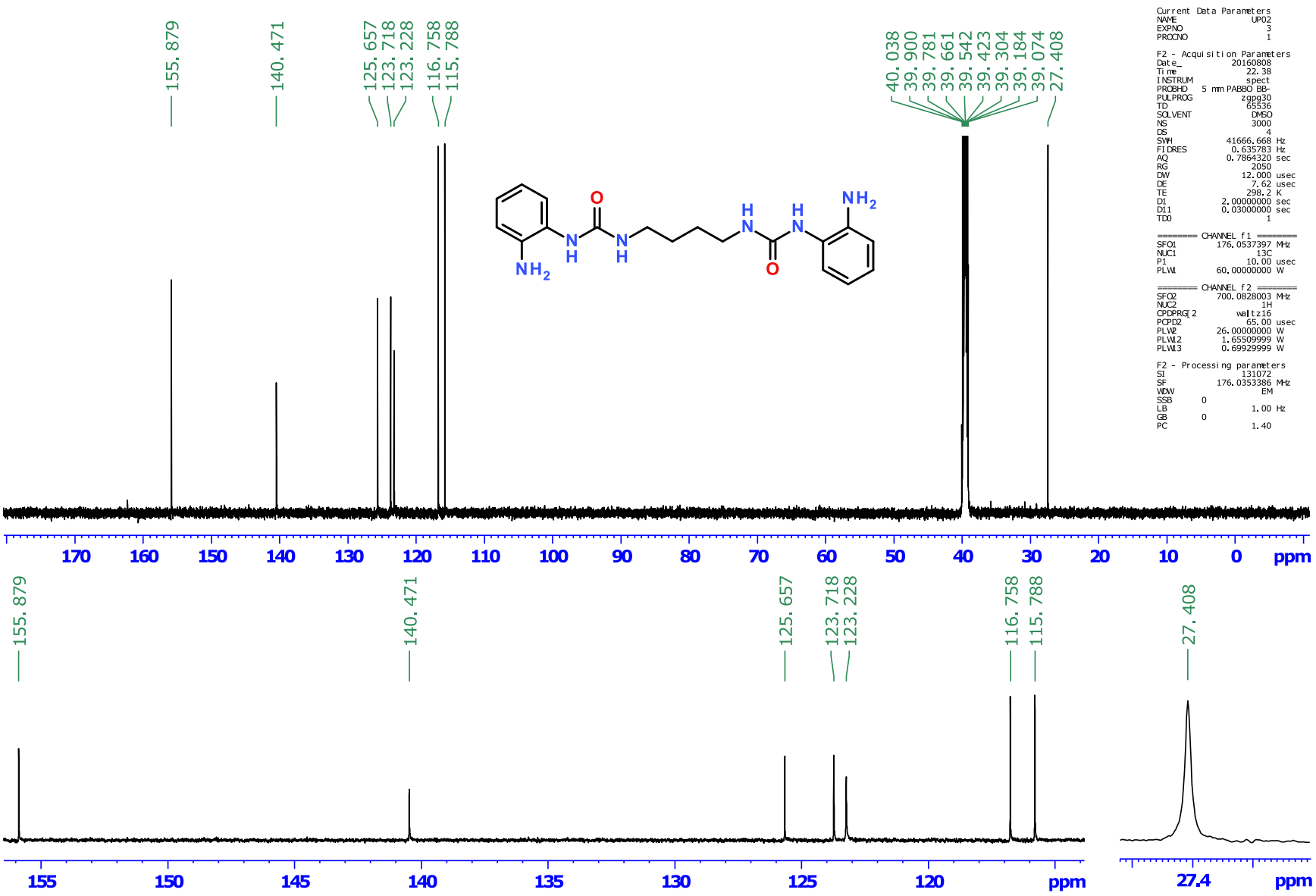
HRMS spectrum of compound U01



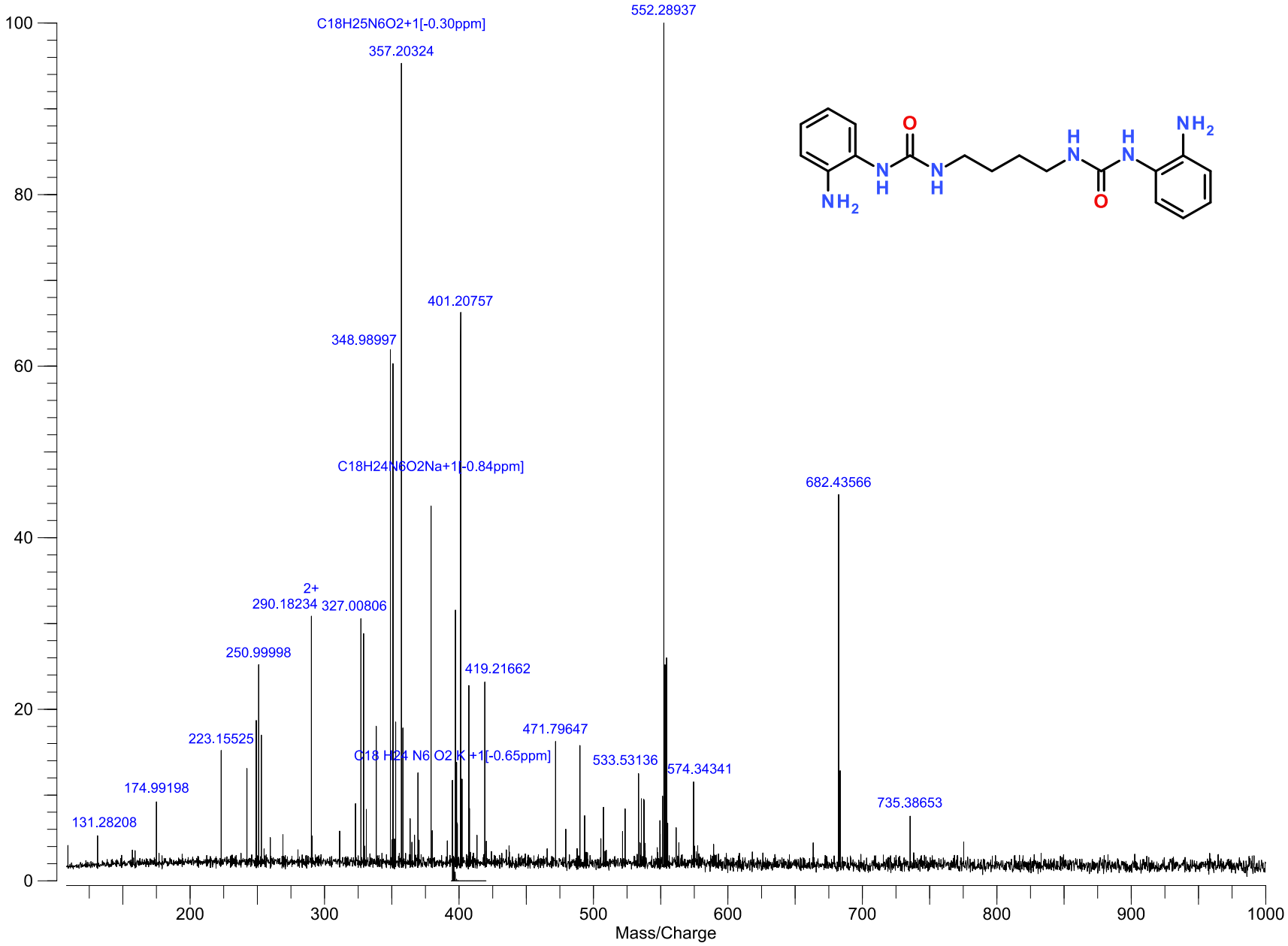
^{1}H NMR spectrum of compound U02



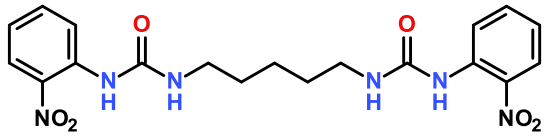
^{13}C NMR spectrum of compound U02

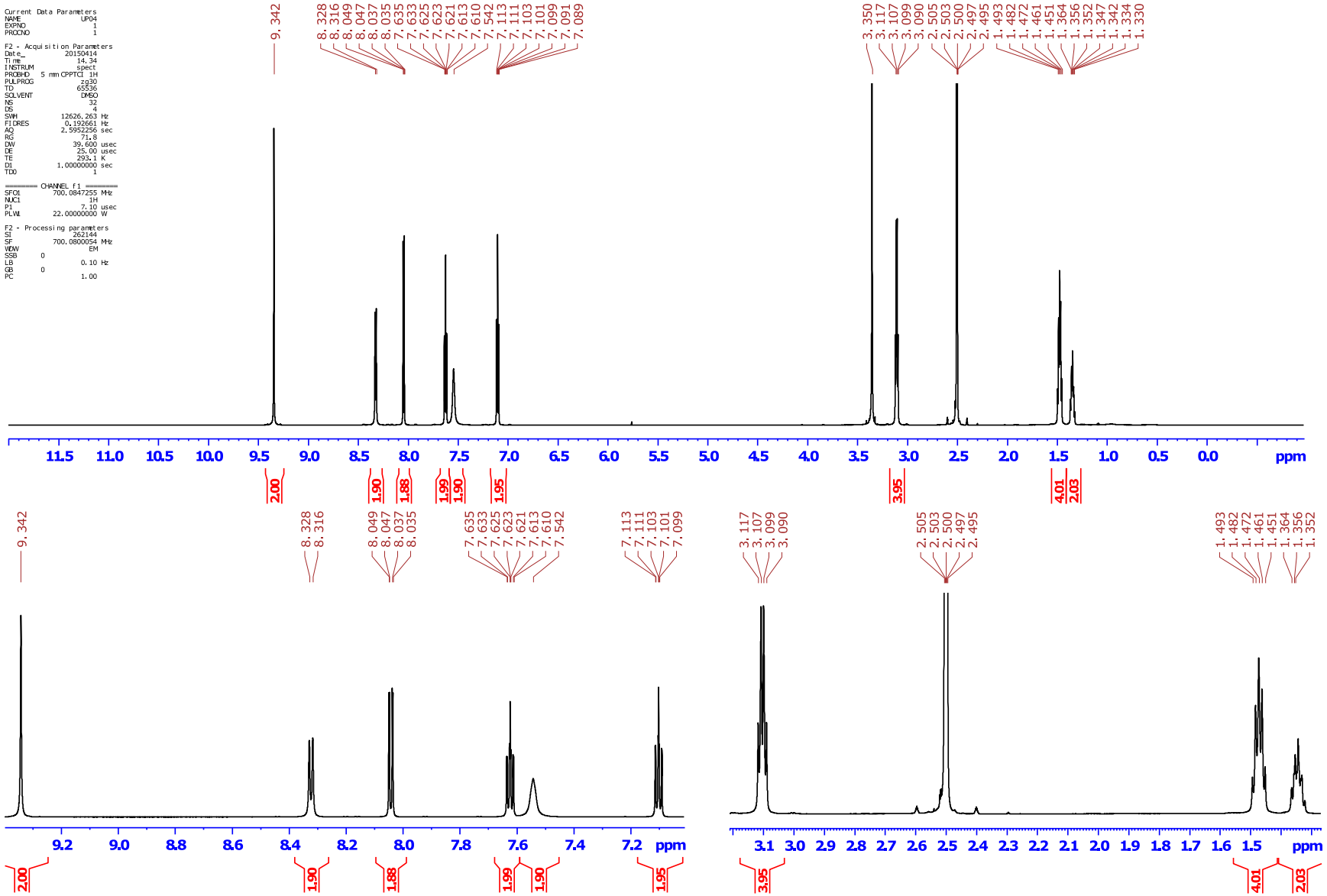


HRMS spectrum of compound U02

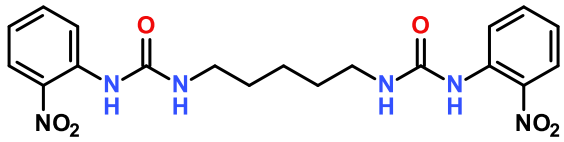


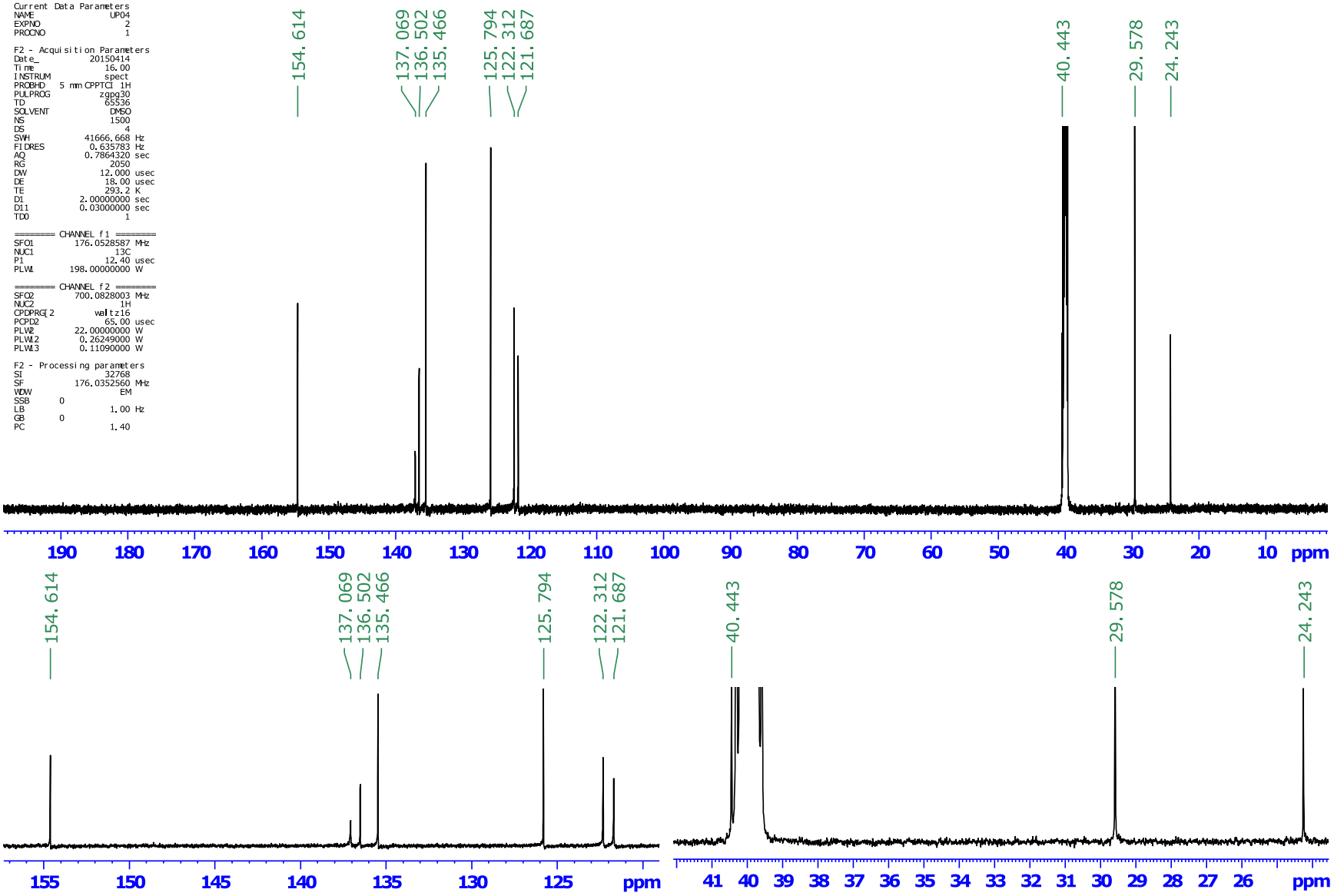
^{1}H NMR spectrum of compound U03



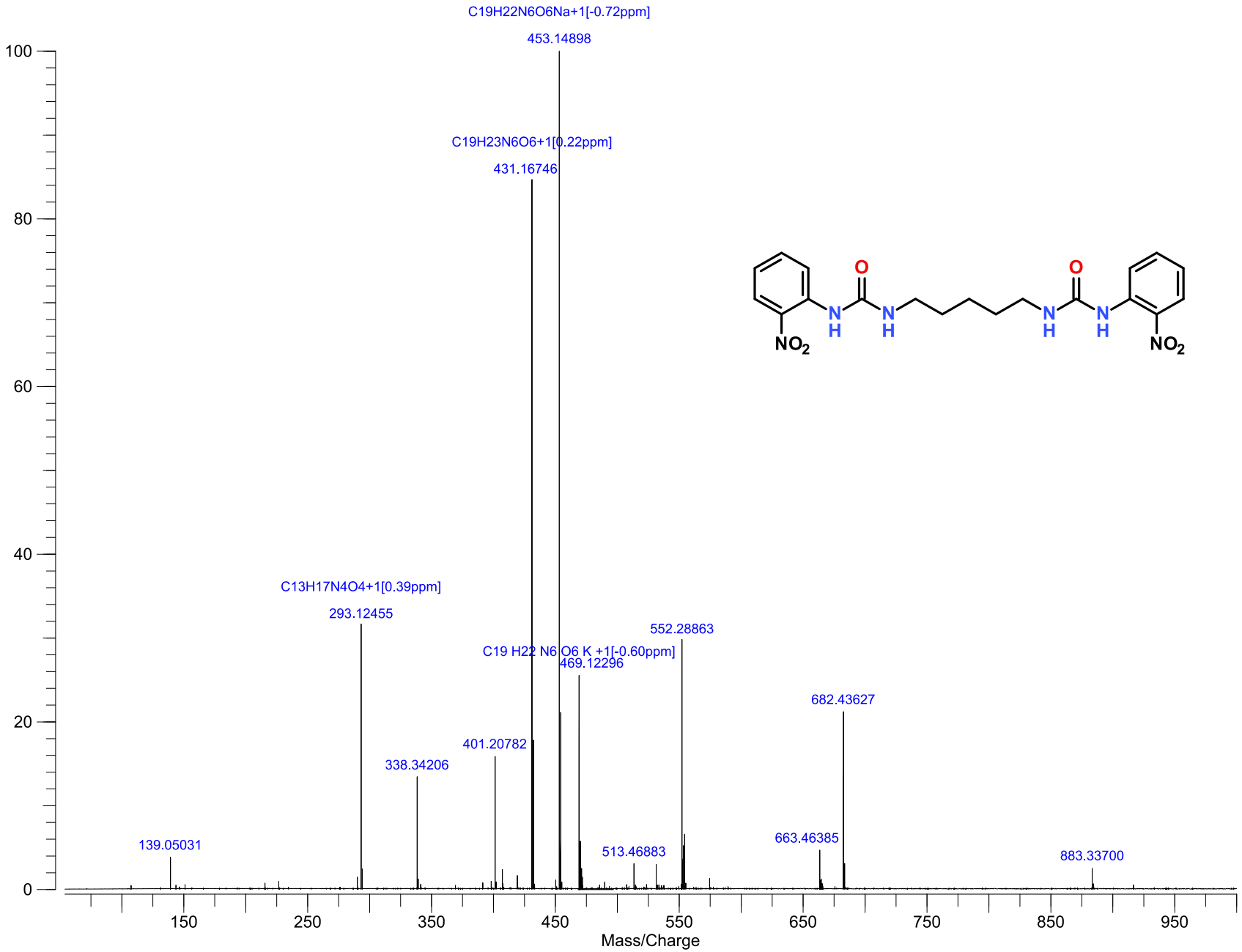


^{13}C NMR spectrum of compound U03

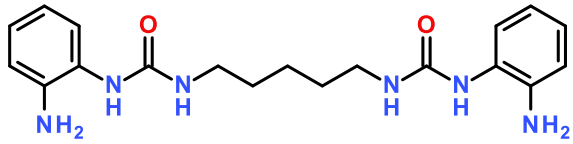


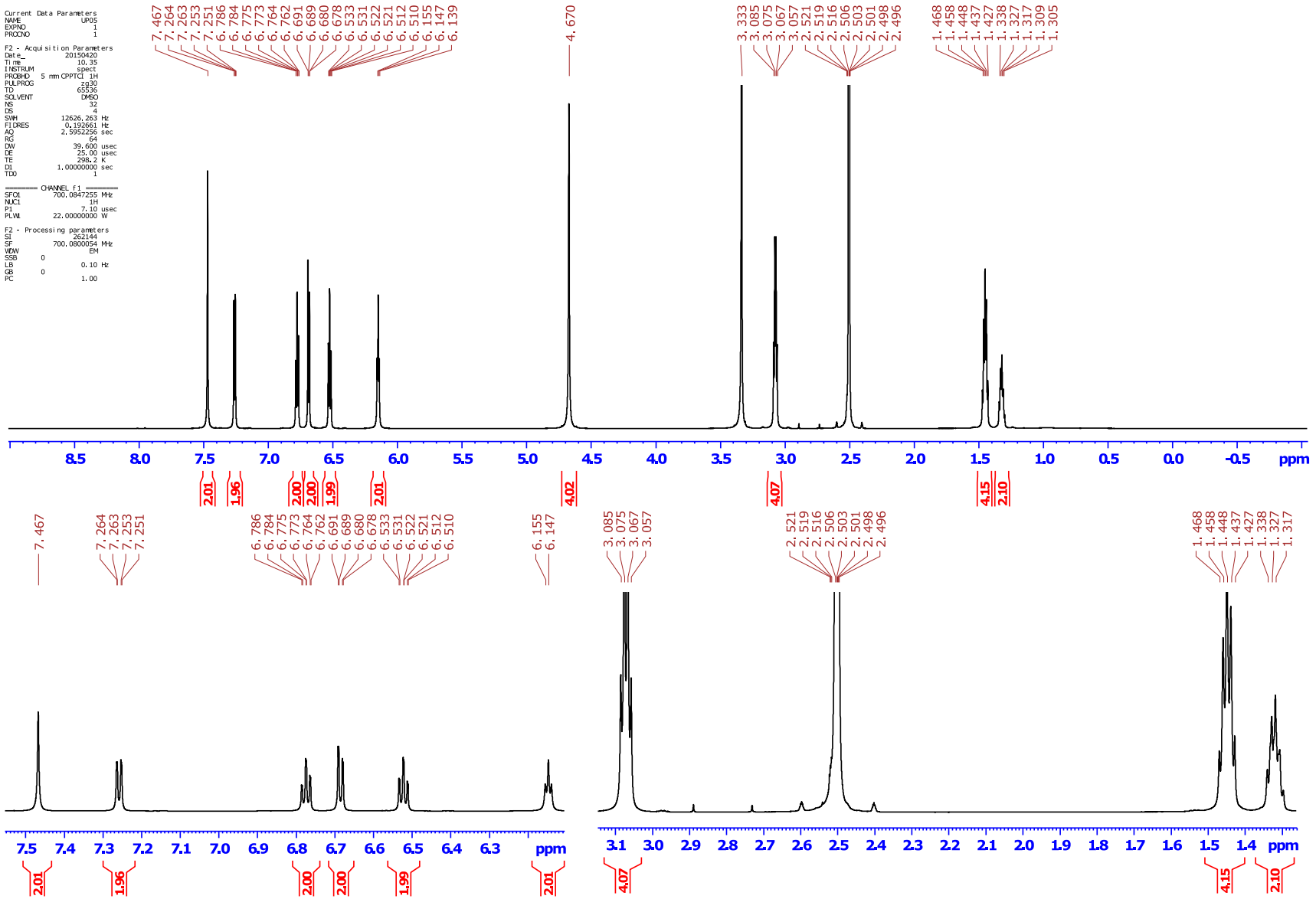


HRMS spectrum of compound U03

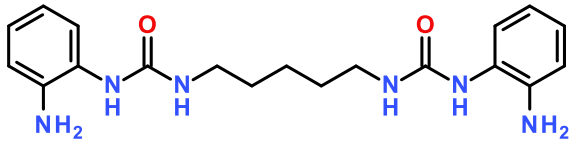


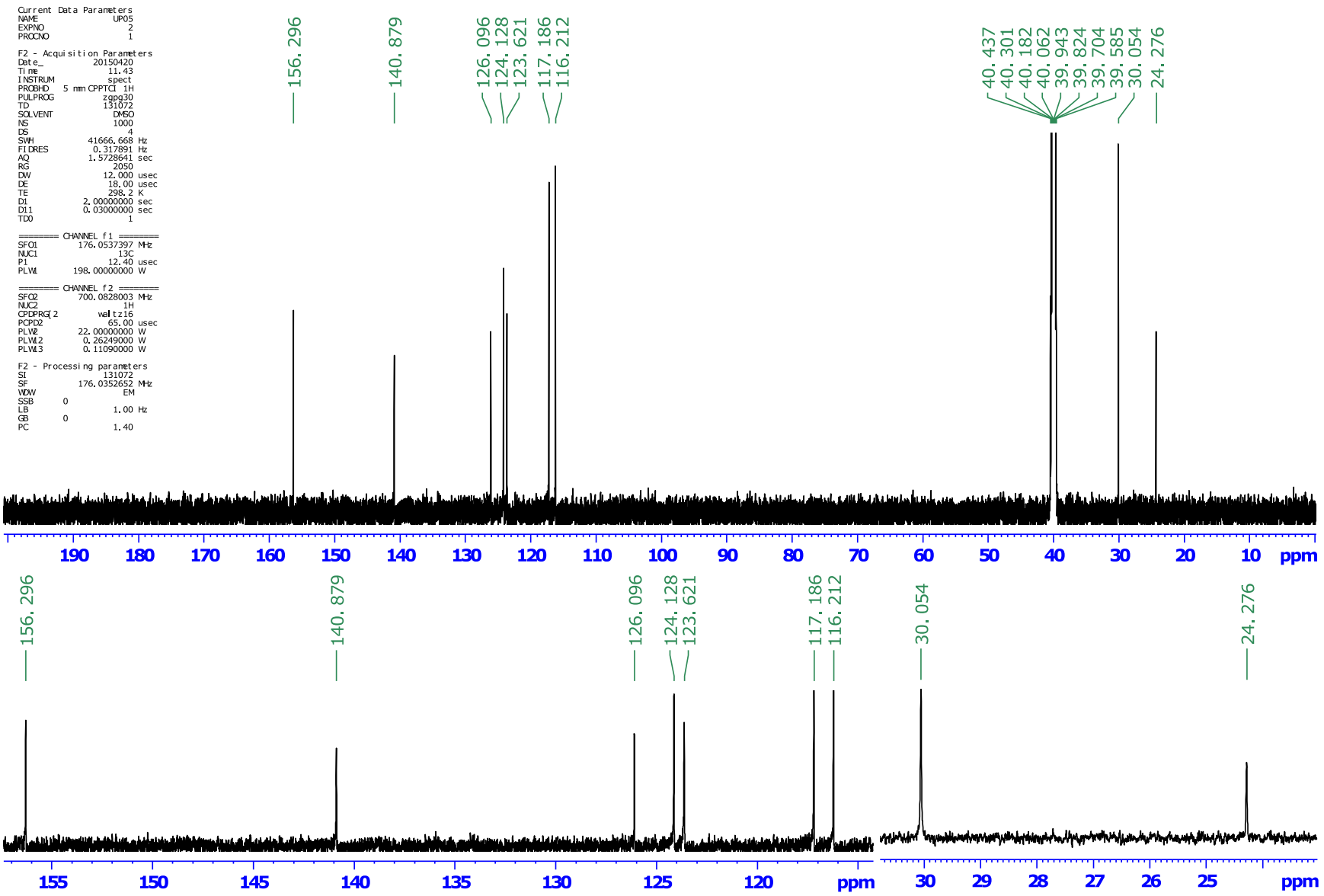
^{1}H NMR spectrum of compound U04



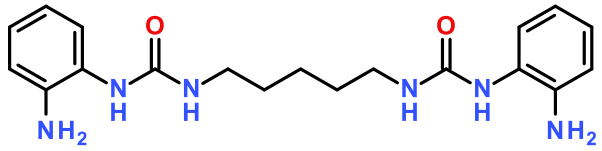


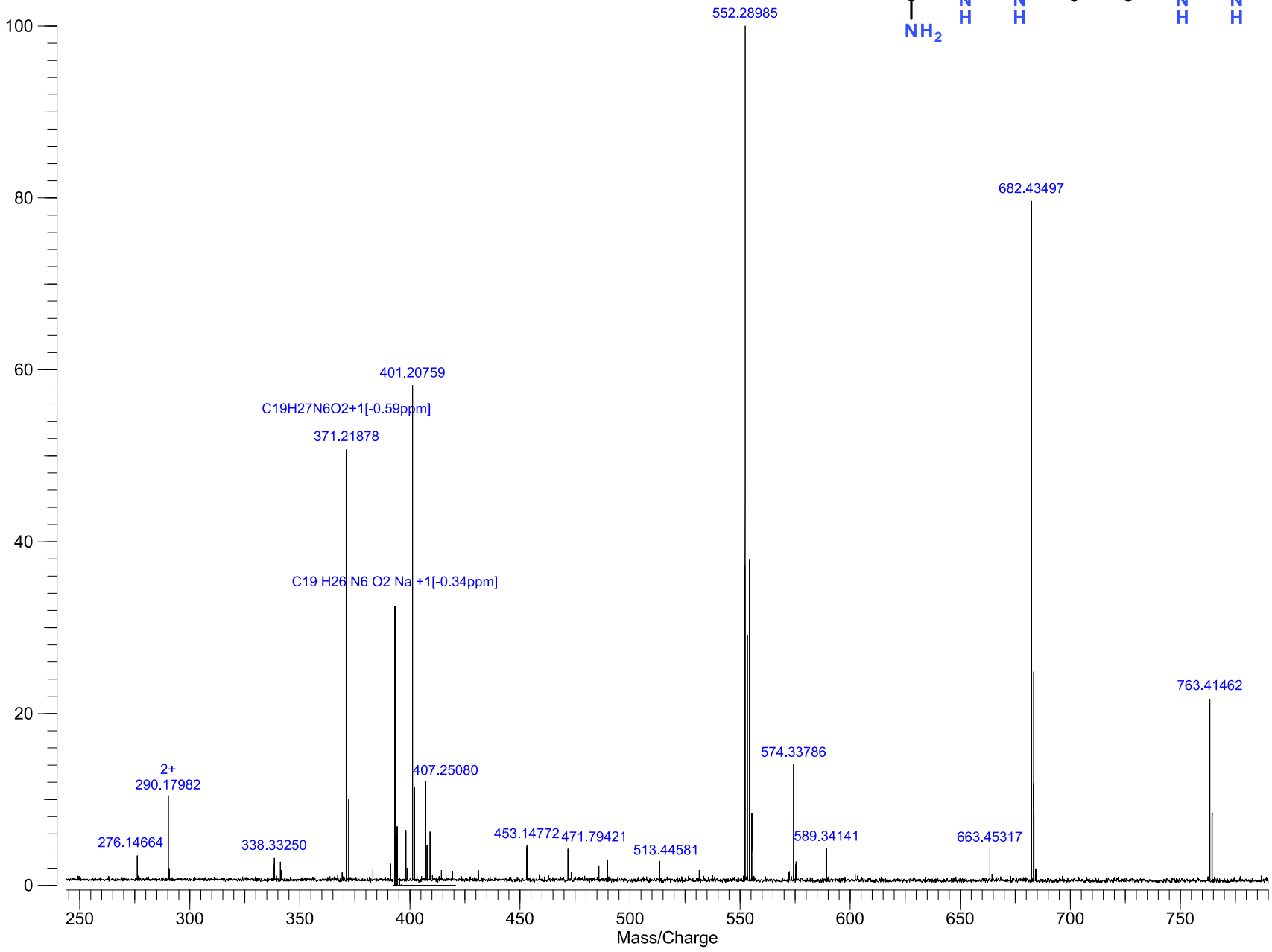
^{13}C NMR spectrum of compound U04



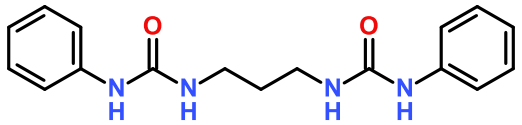


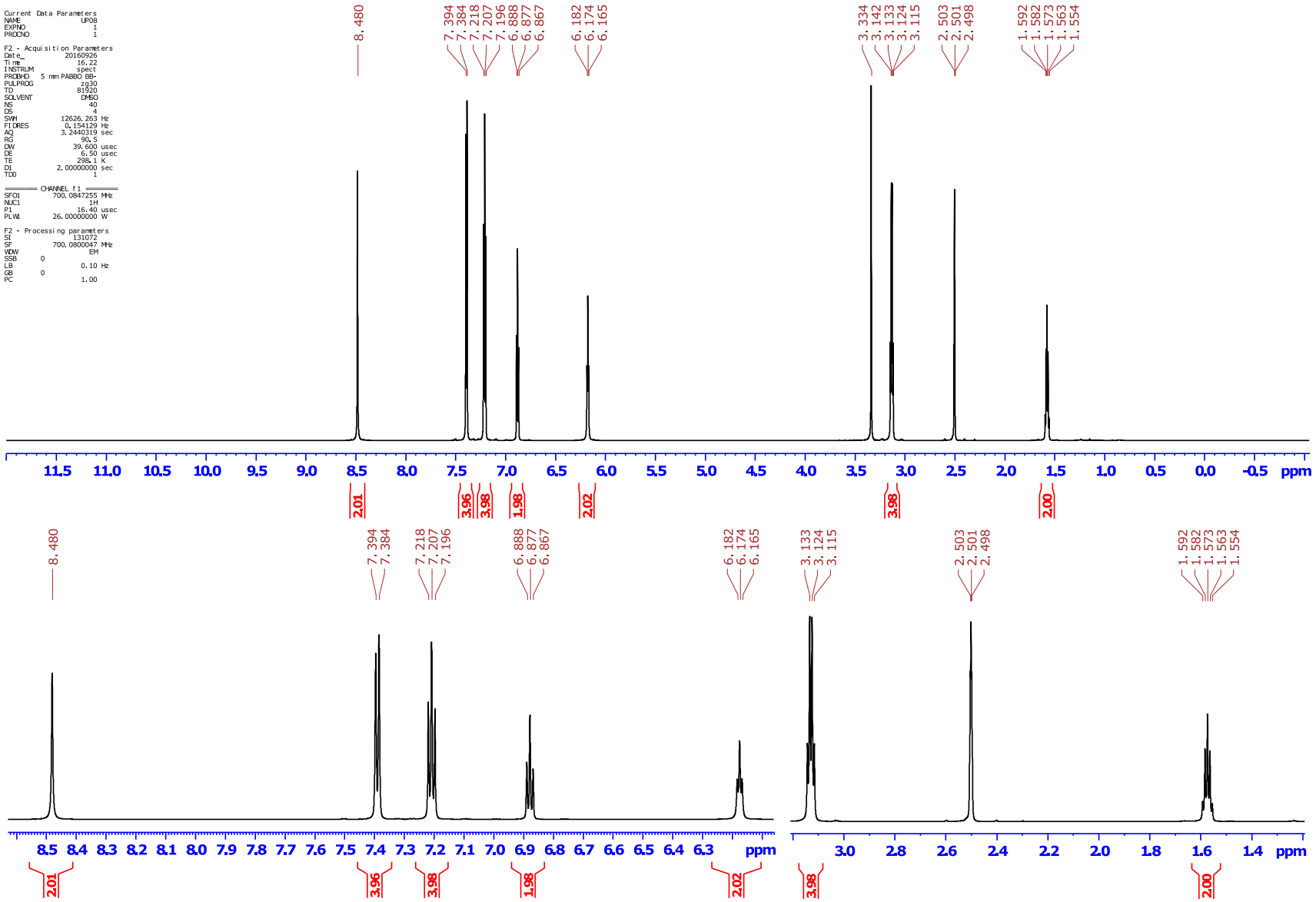
HRMS spectrum of compound U04



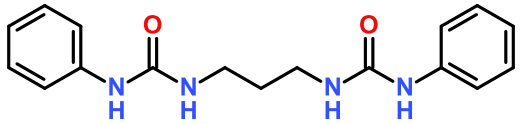


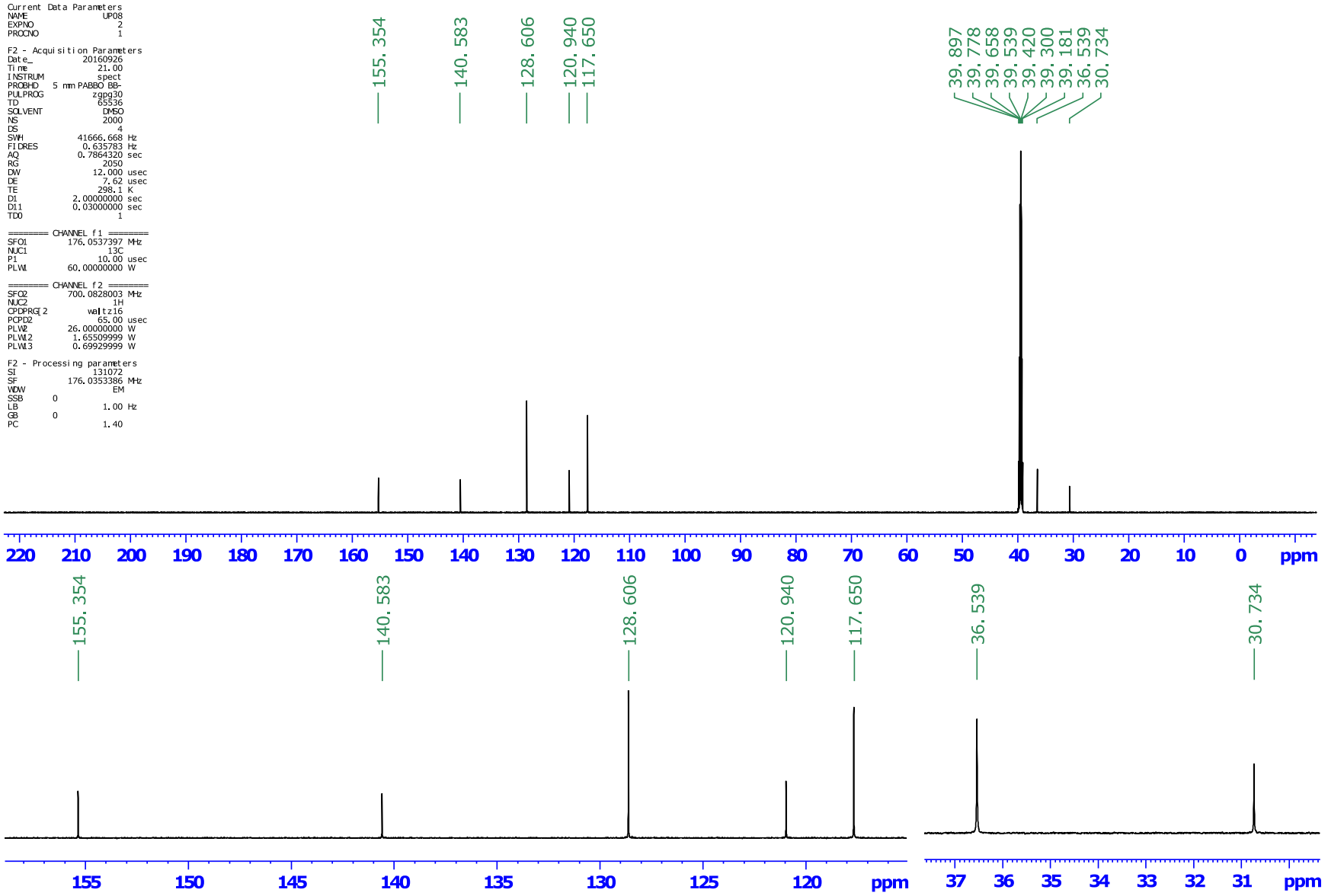
^{1}H NMR spectrum of compound U05



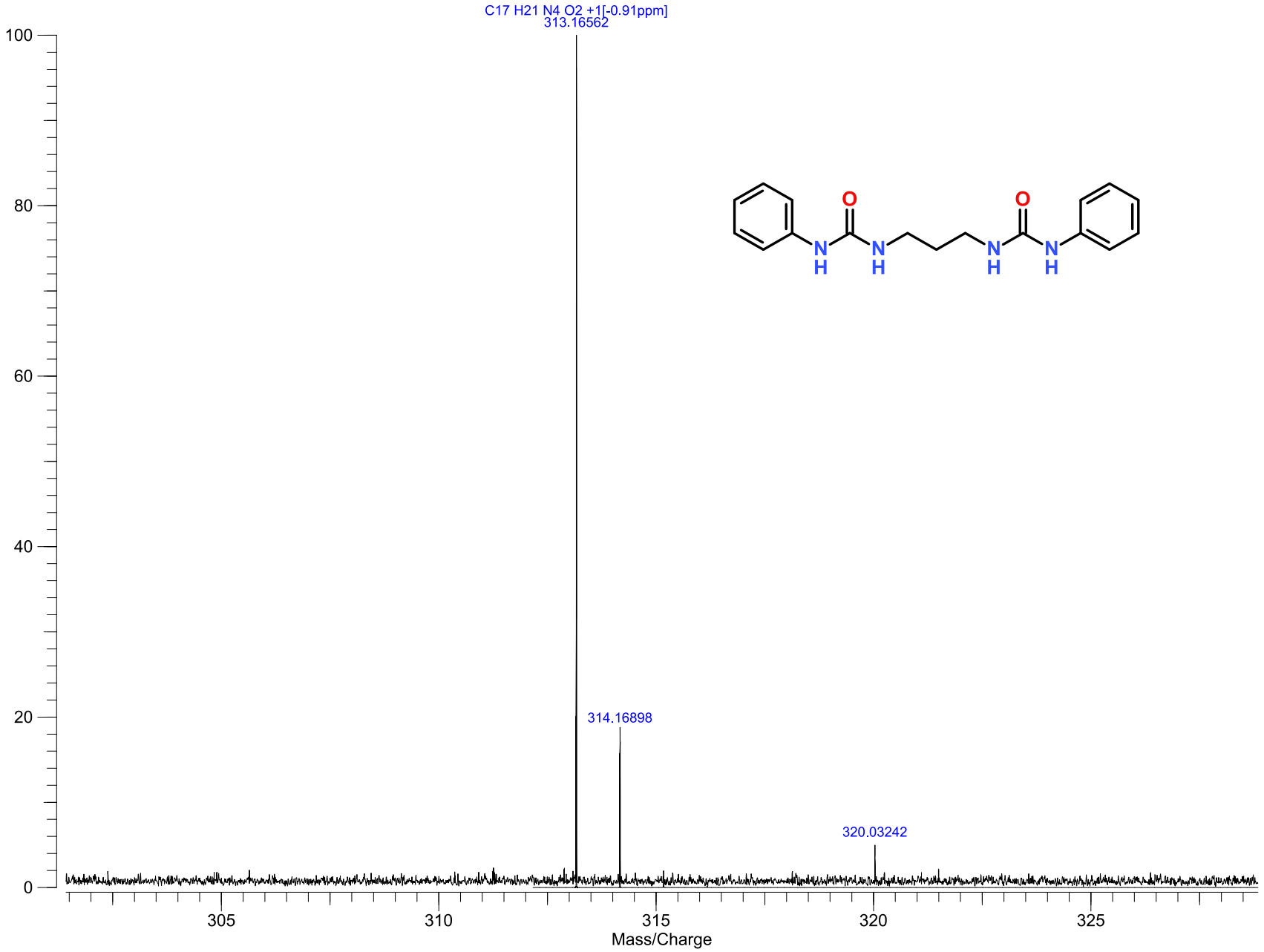


^{13}C NMR spectrum of compound U05

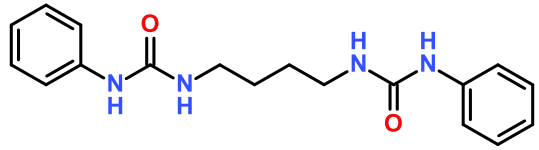


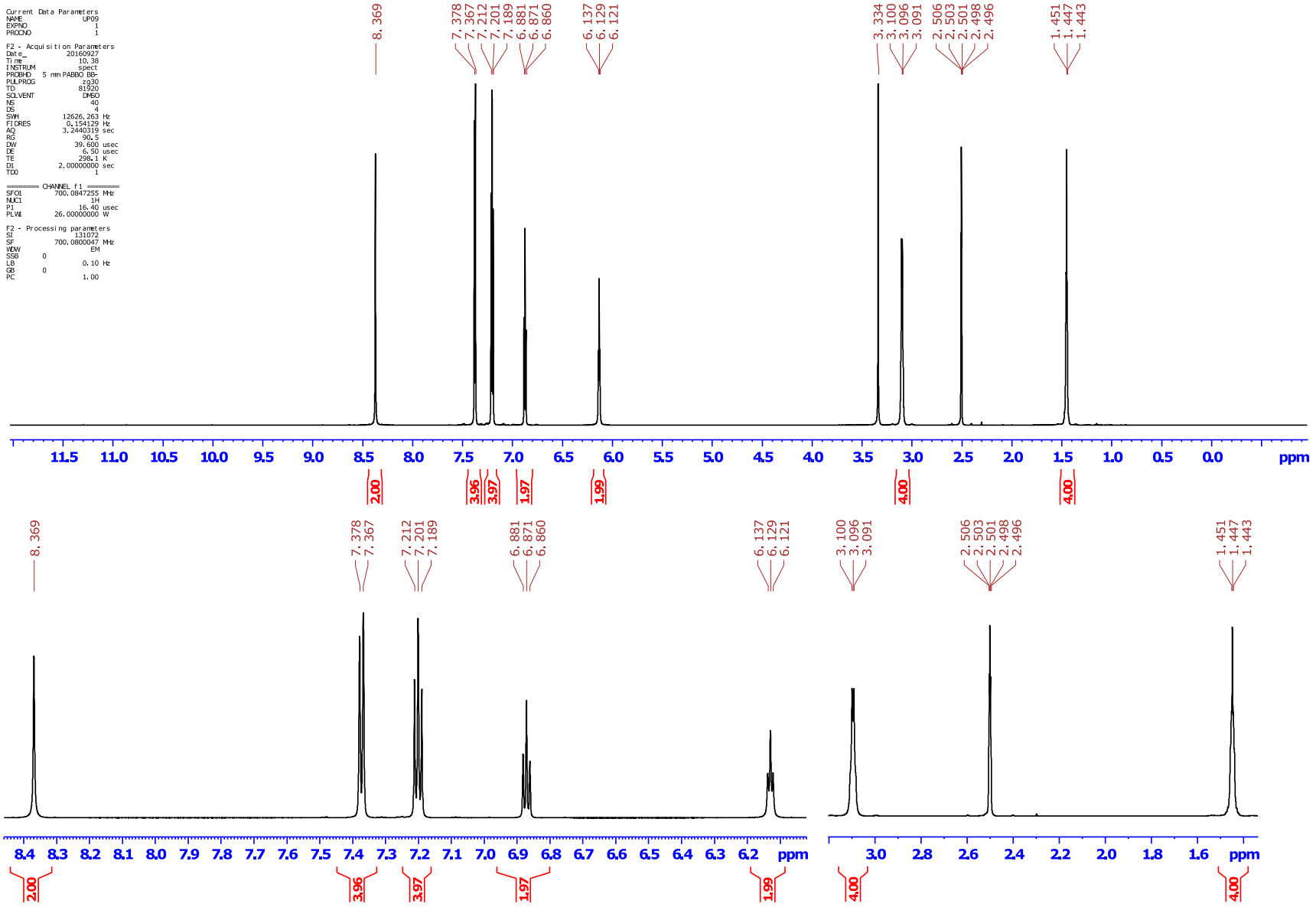


HRMS spectrum of compound U05

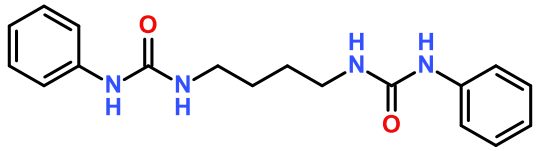


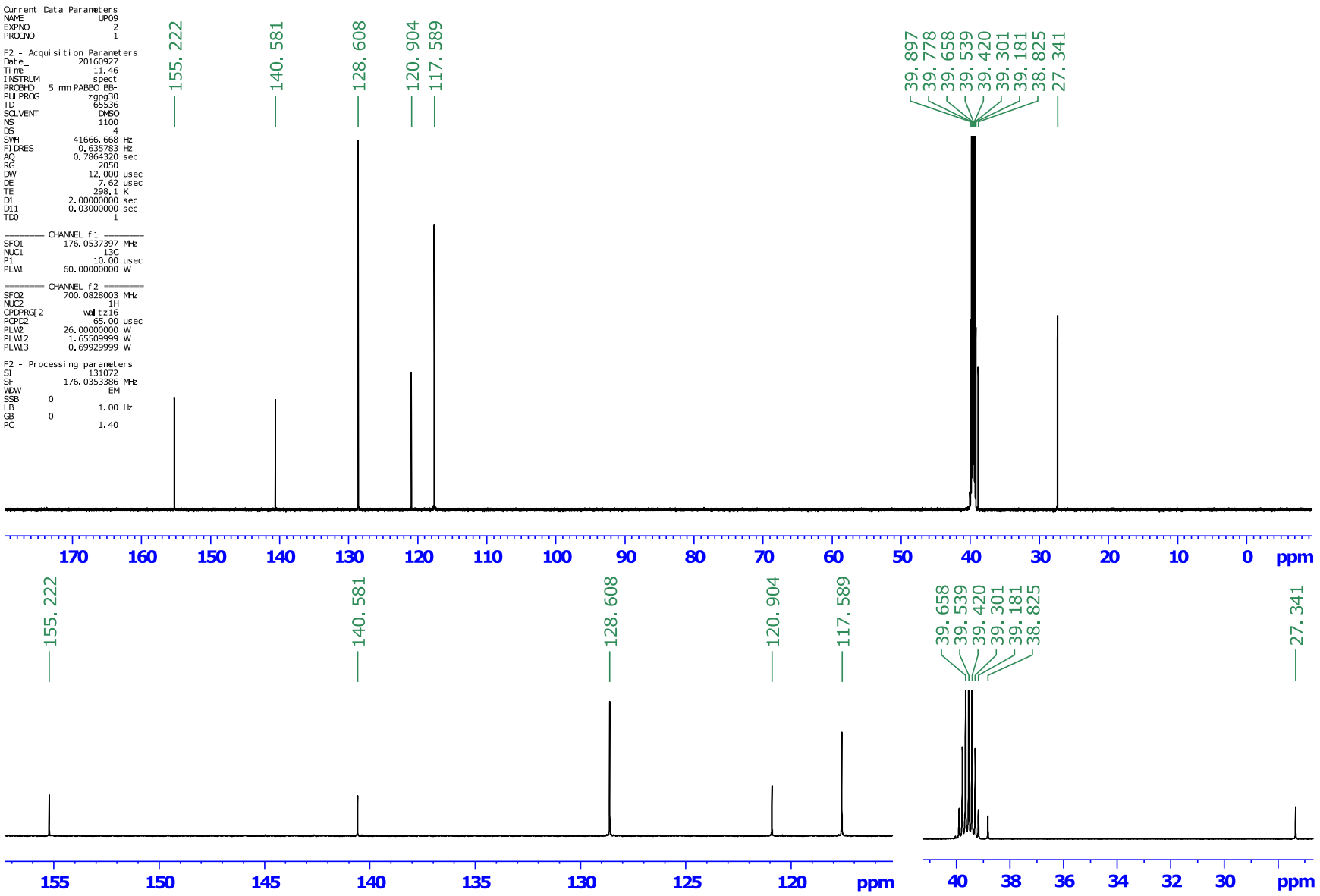
^{1}H NMR spectrum of compound U06



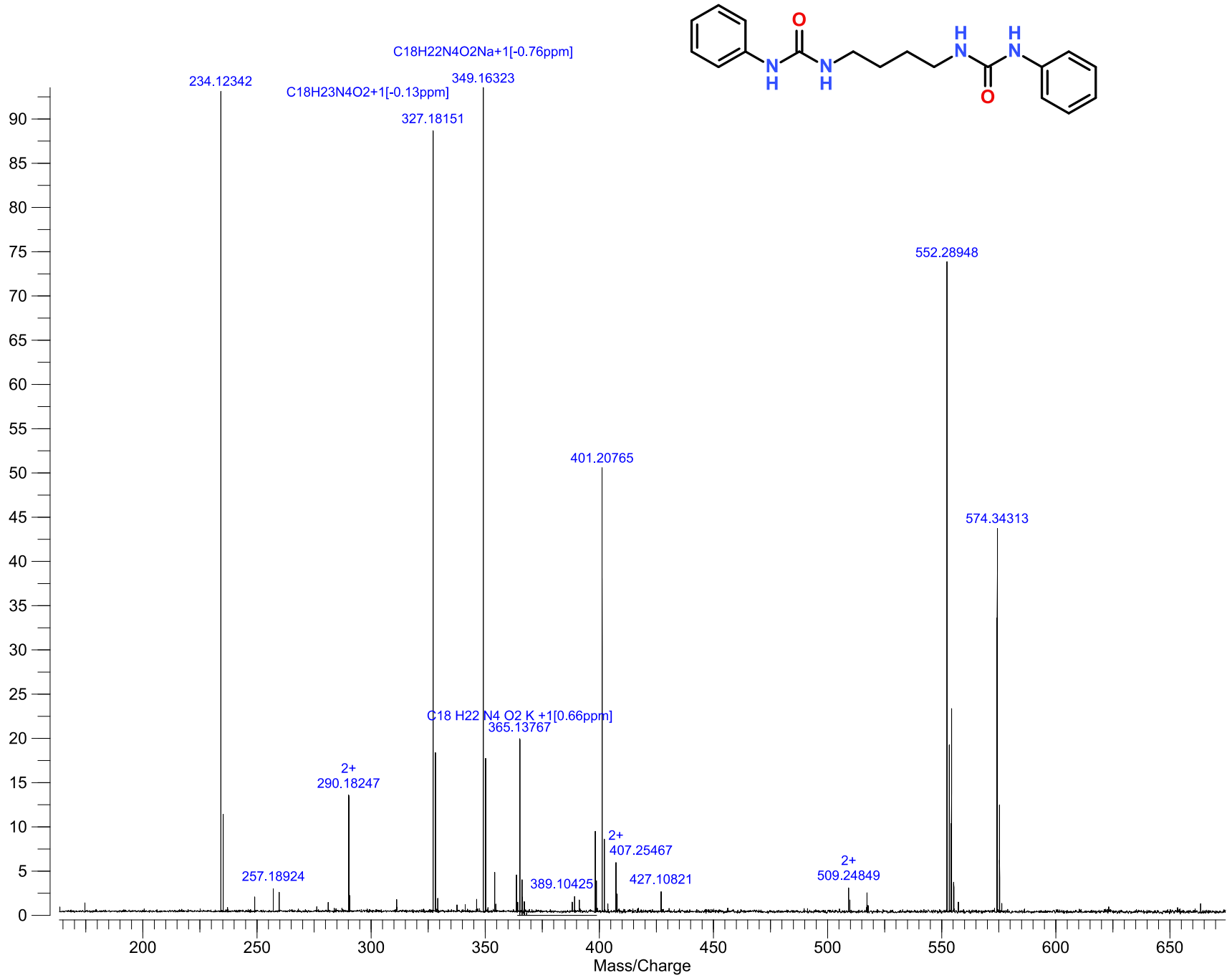


^{13}C NMR spectrum of compound U06

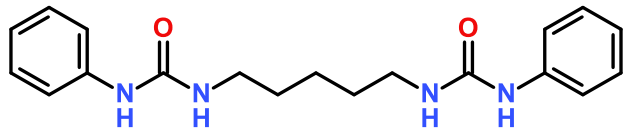


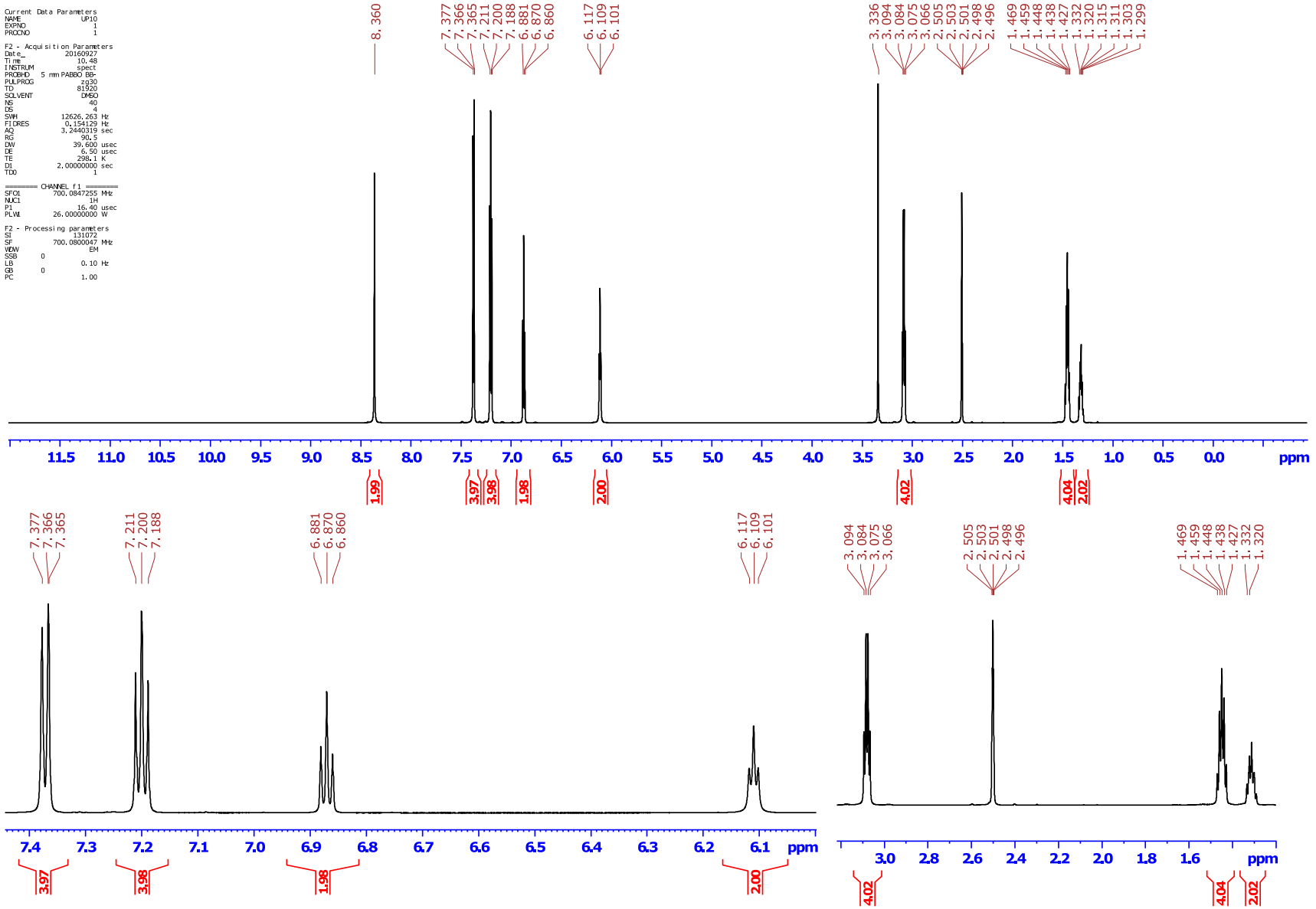


HRMS spectrum of compound U06

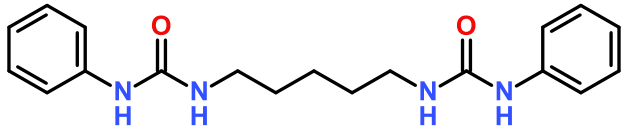


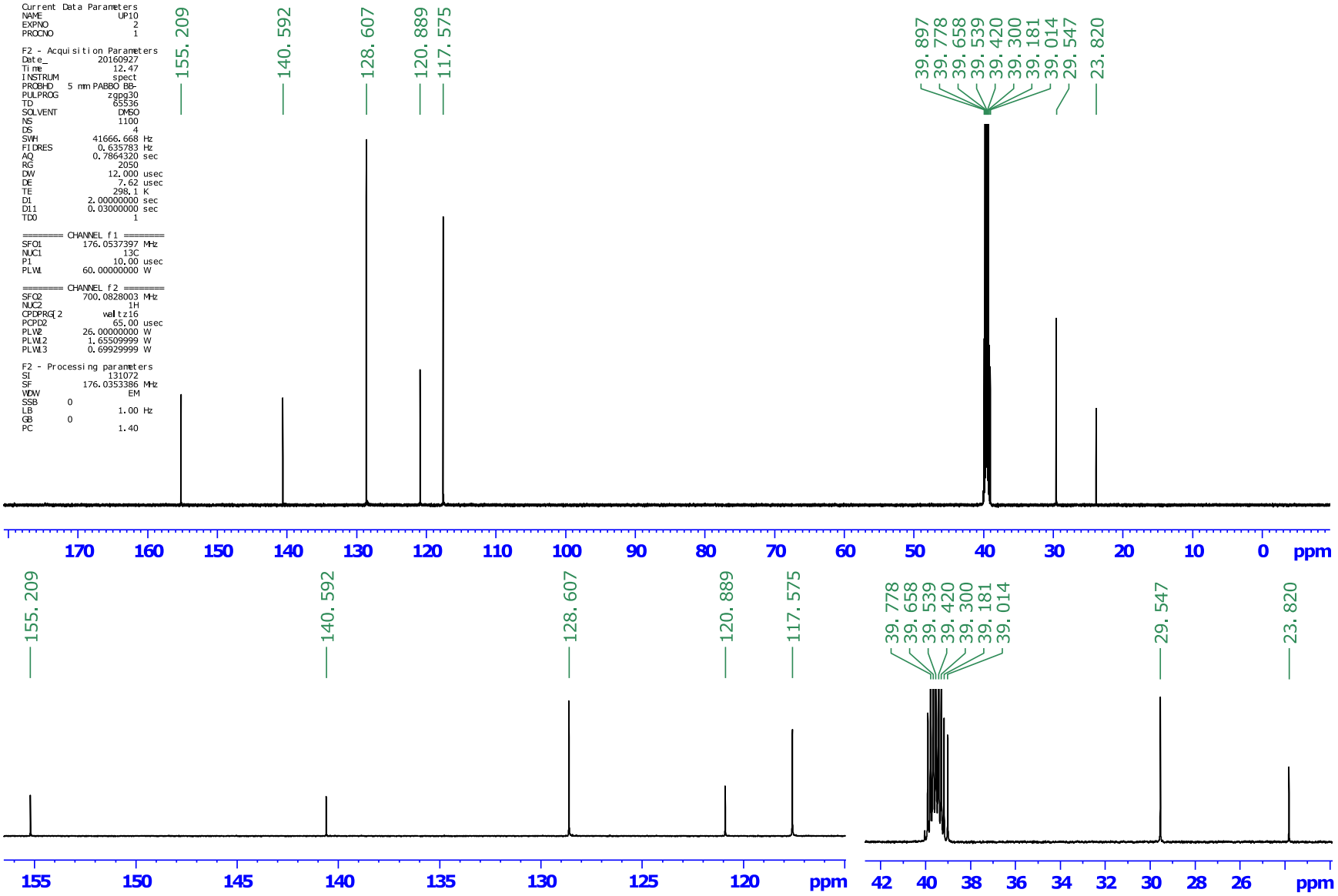
^{1}H NMR spectrum of compound U07



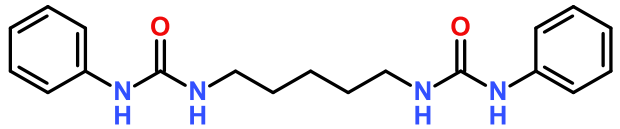


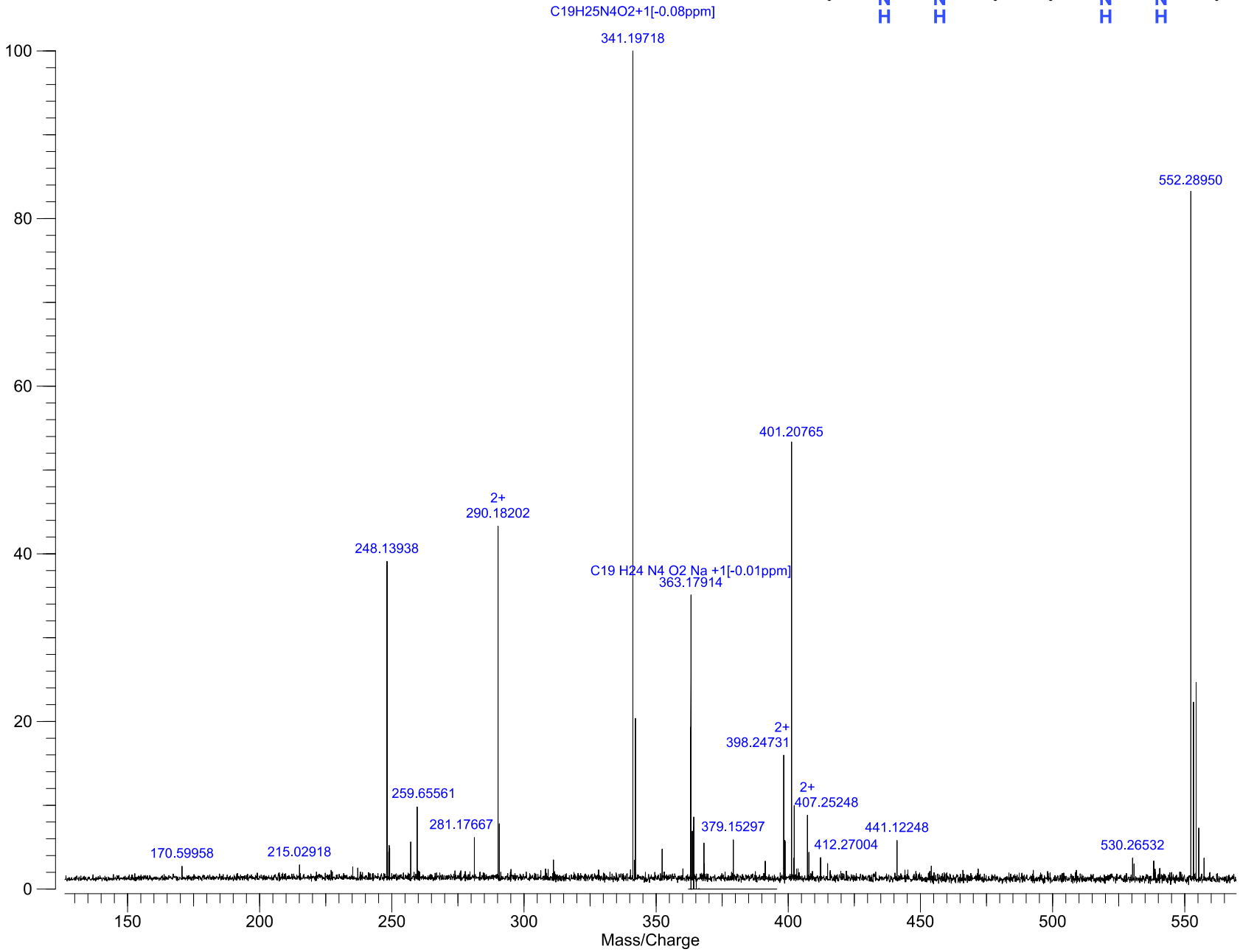
^{13}C NMR spectrum of compound U07



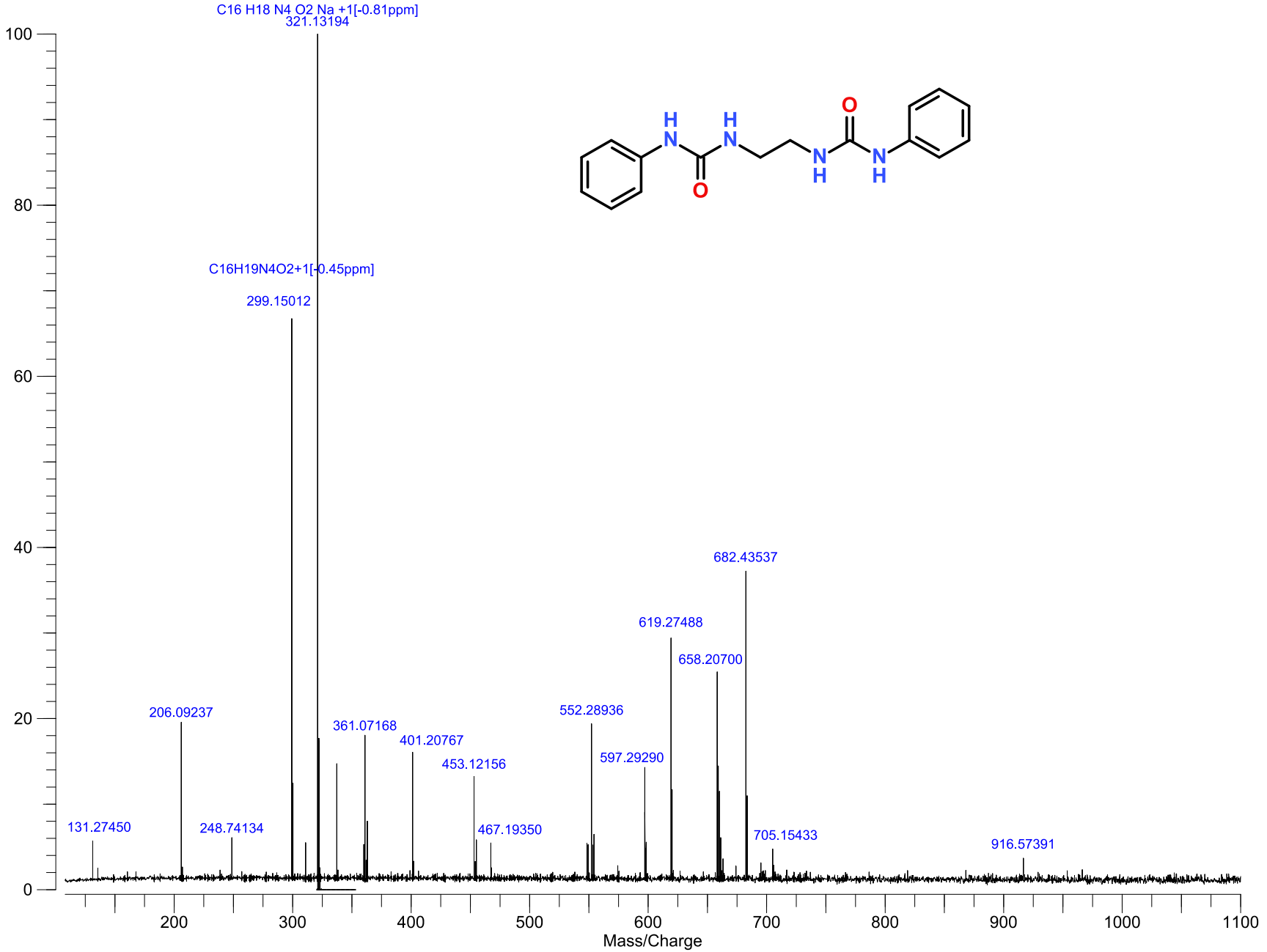


HRMS spectrum of compound U07

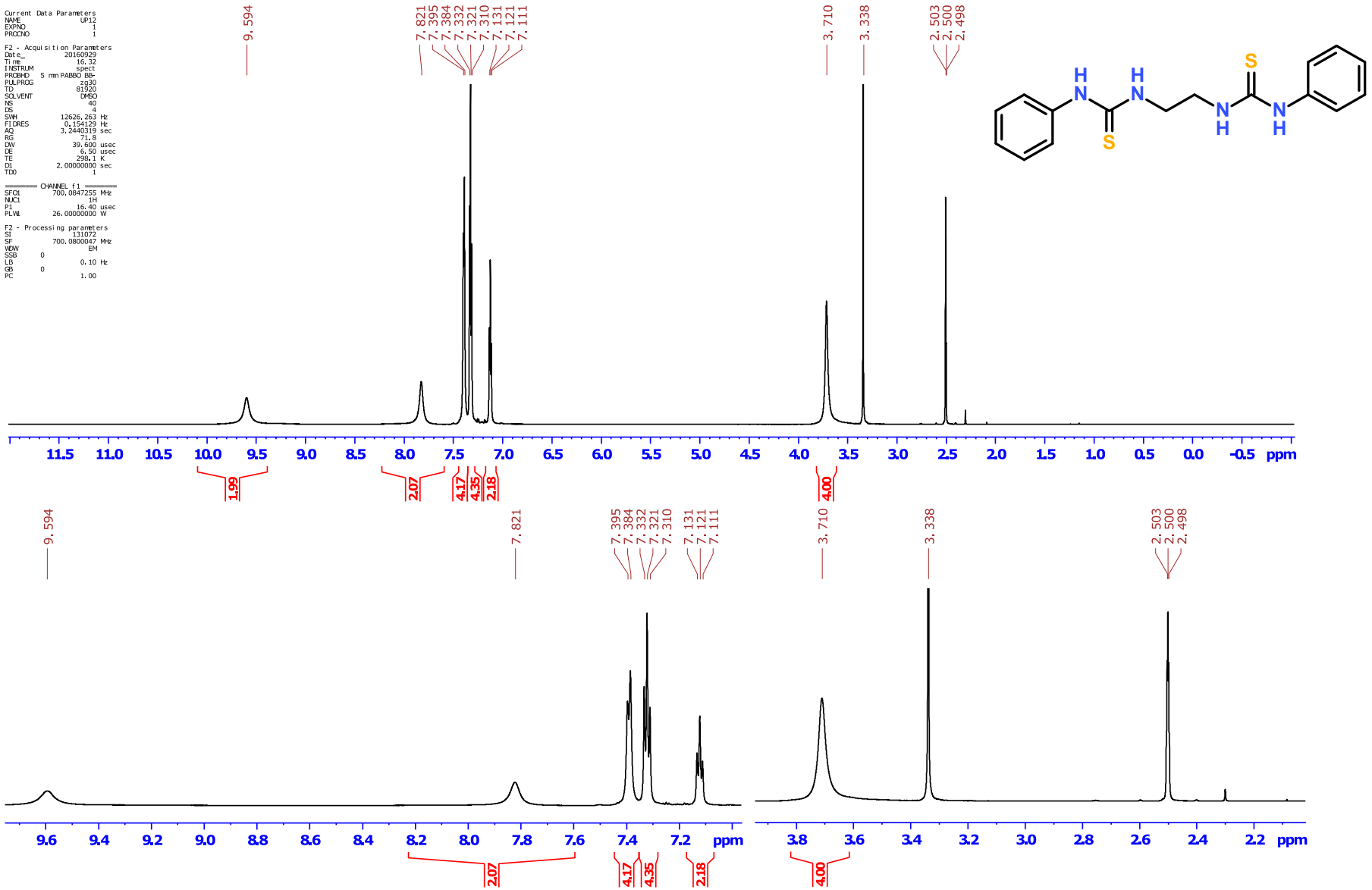




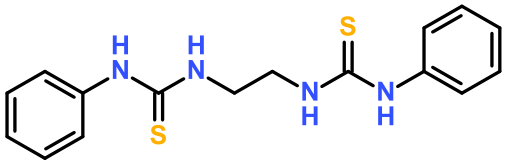
HRMS spectrum of compound U08

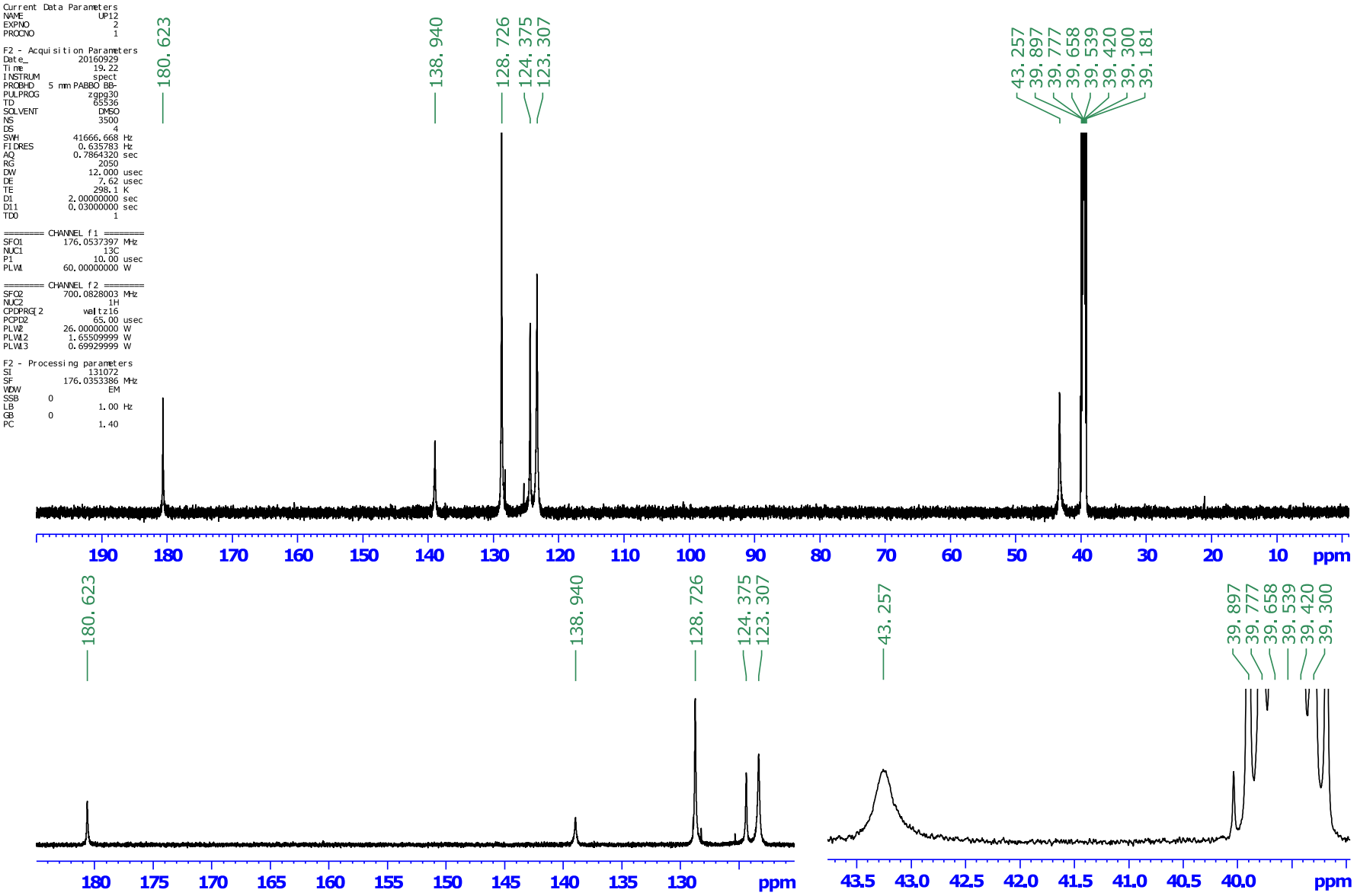


^{1}H NMR spectrum of compound U09

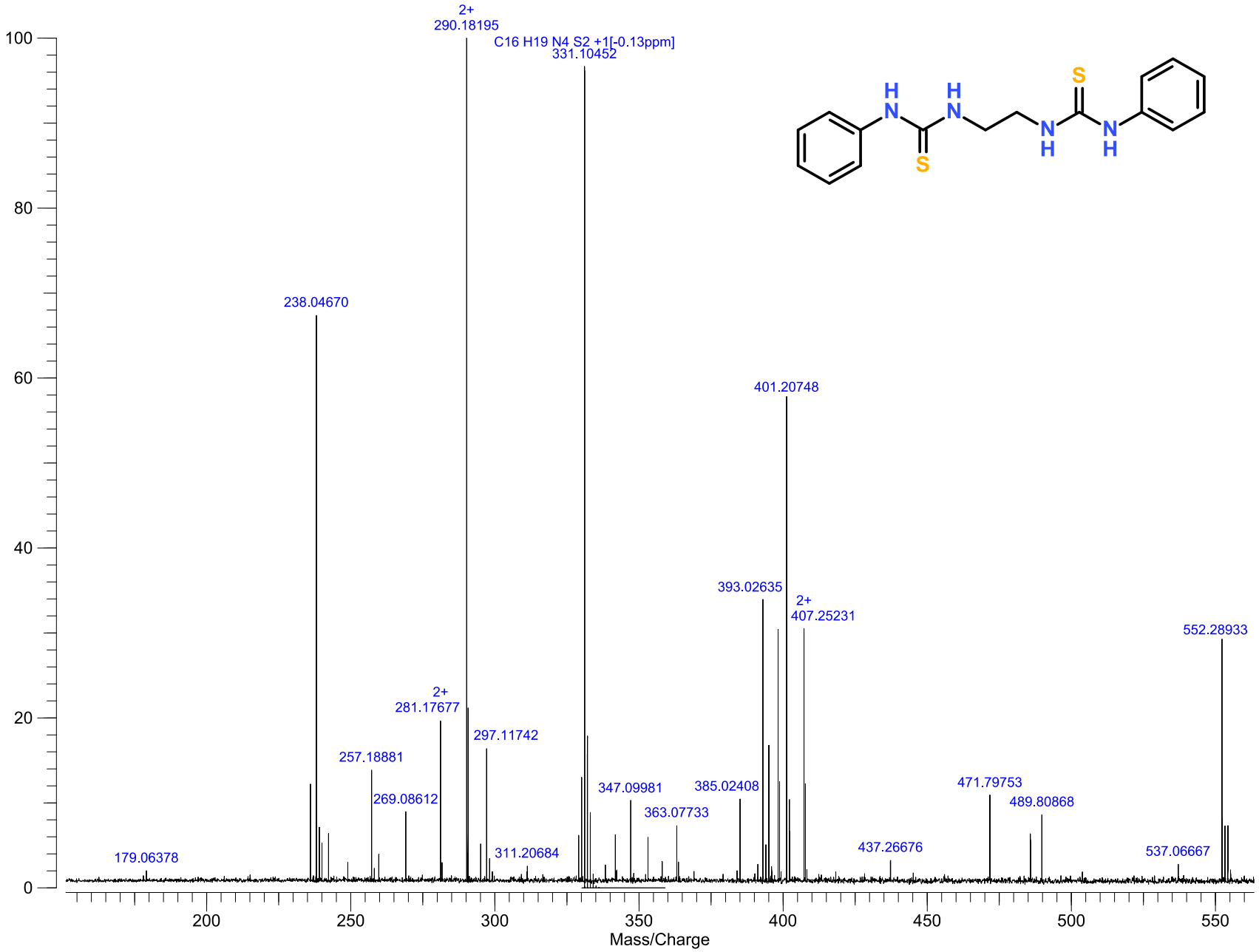


^{13}C NMR spectrum of compound U09

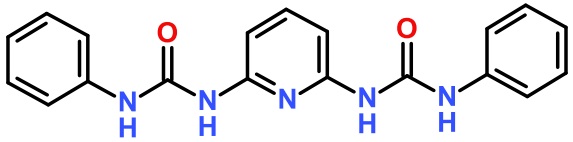


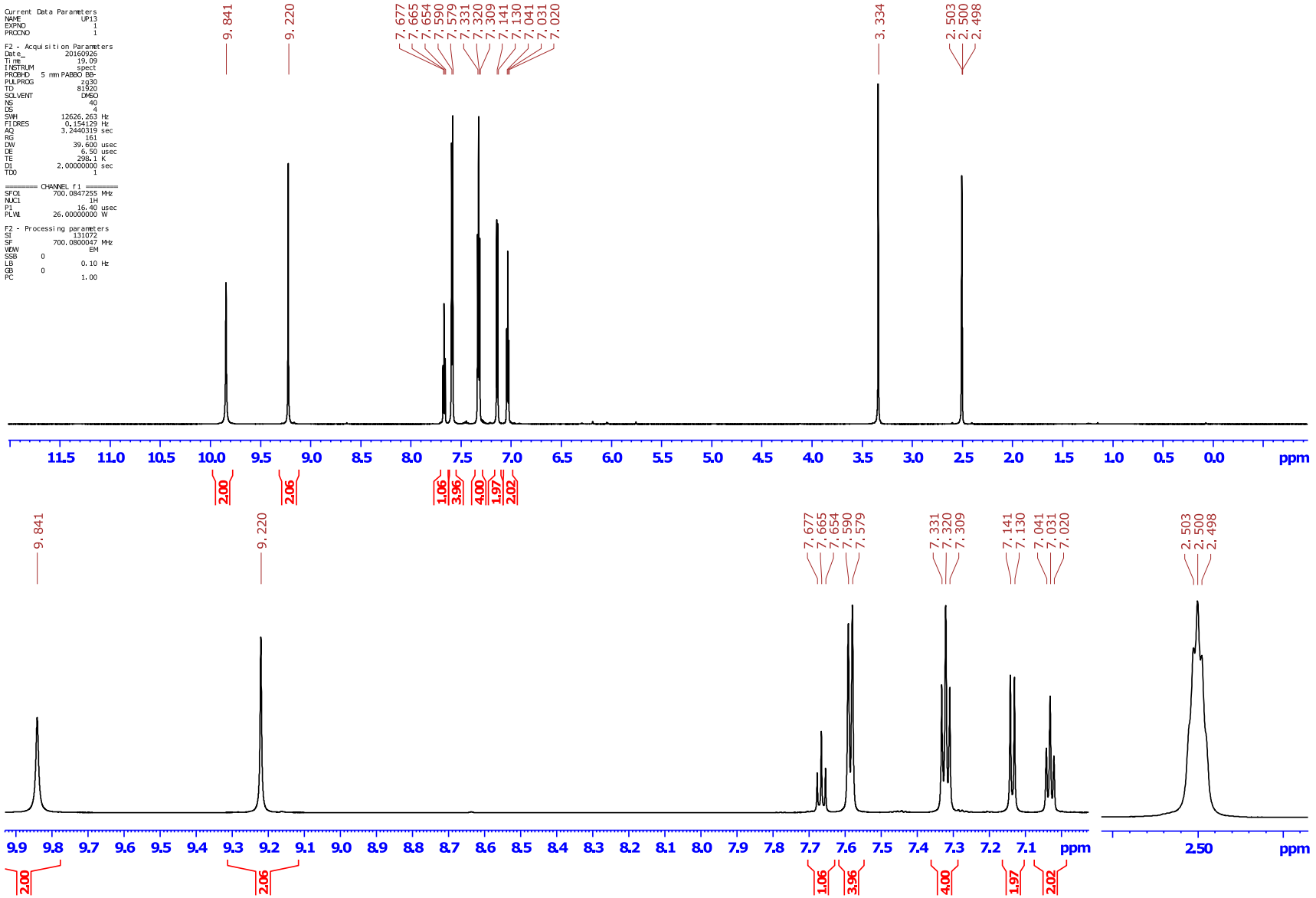


HRMS spectrum of compound U09

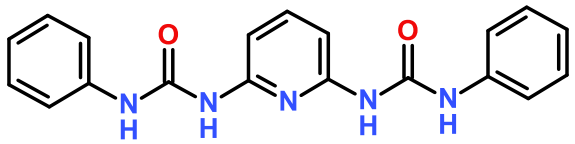


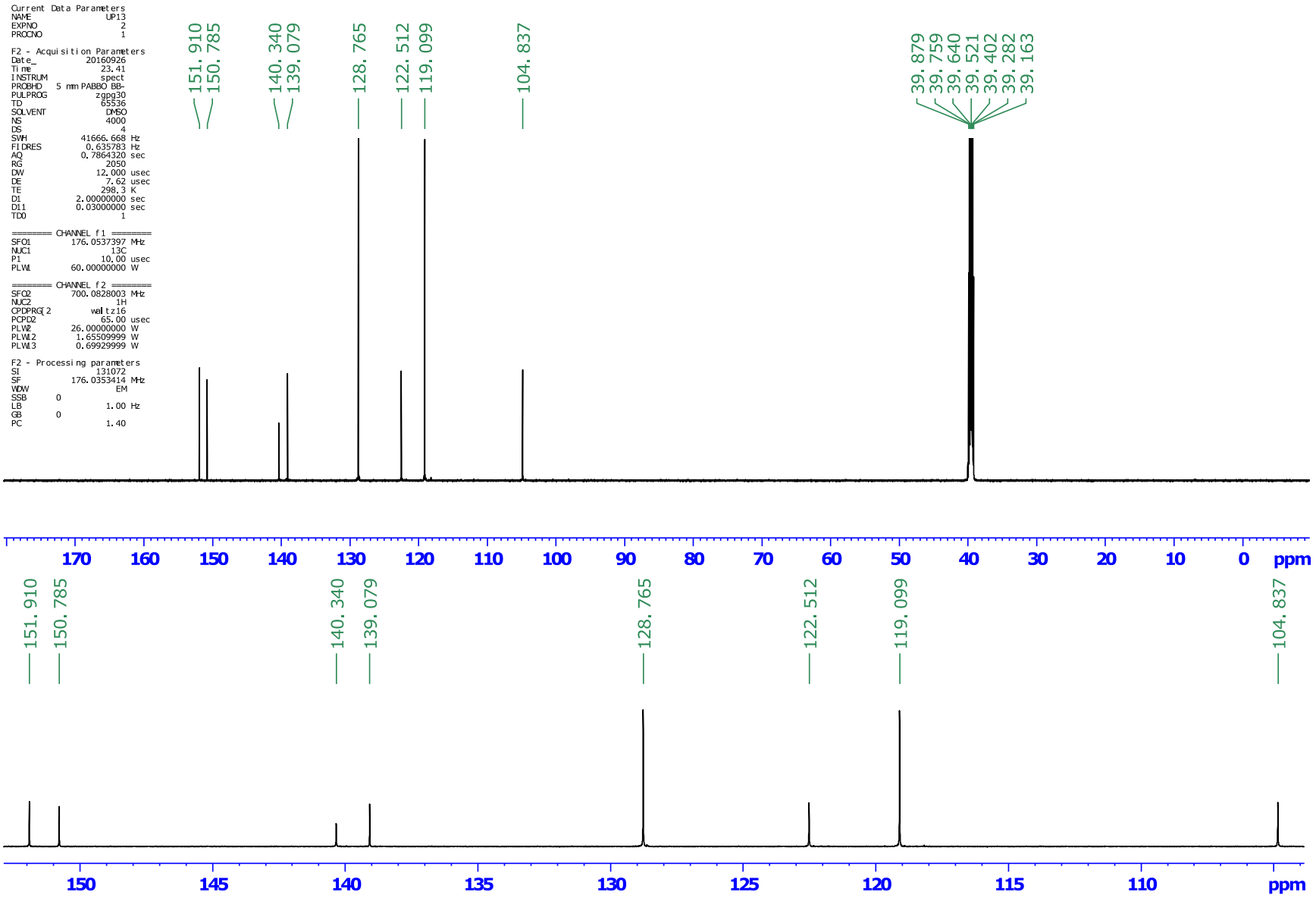
^{1}H NMR spectrum of compound U10



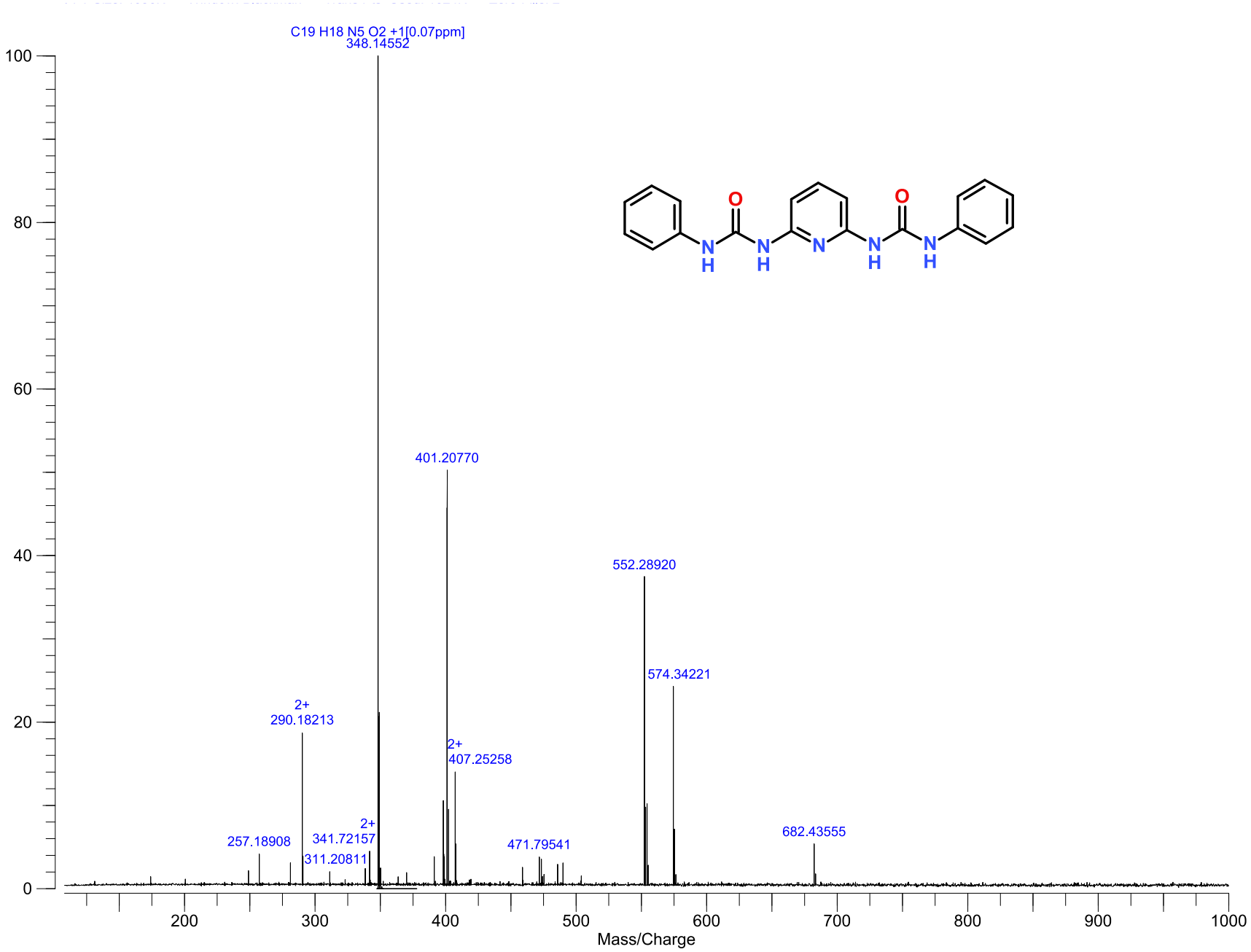


^{13}C NMR spectrum of compound U10

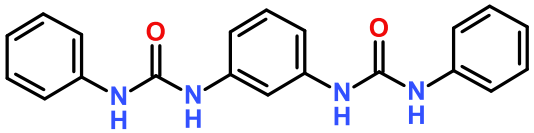


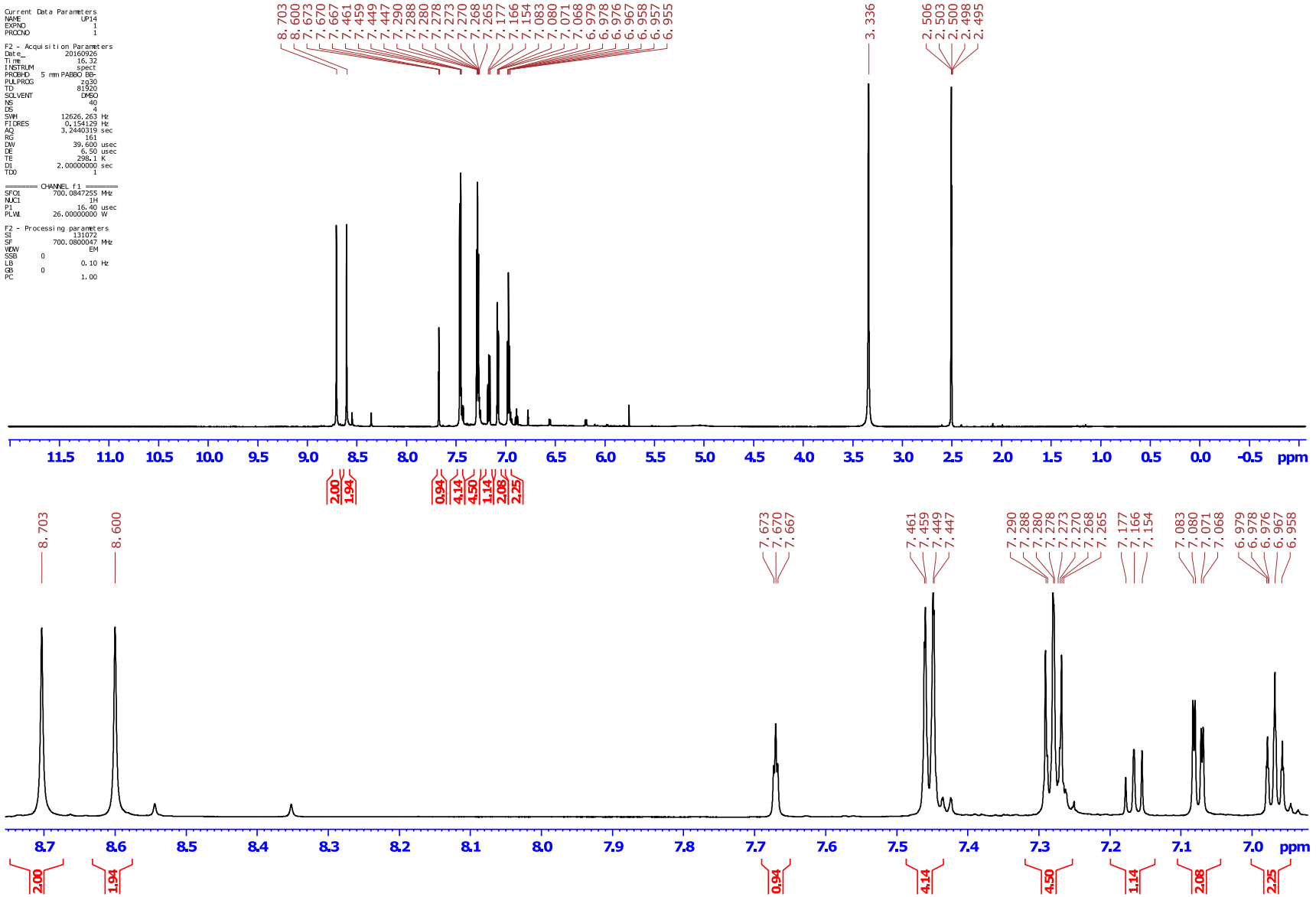


HRMS spectrum of compound U10

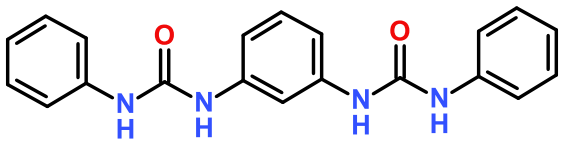


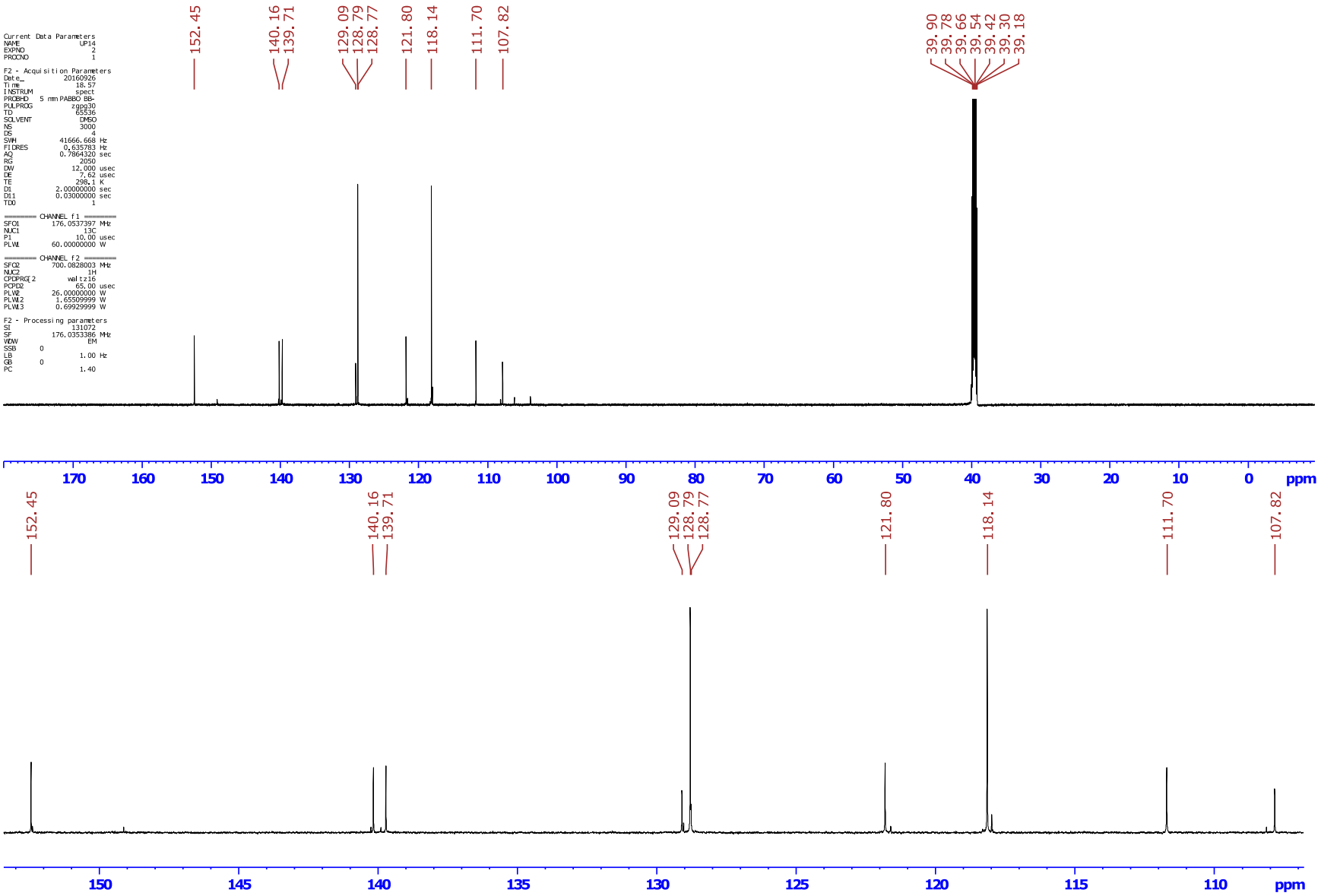
^{1}H NMR spectrum of compound U11



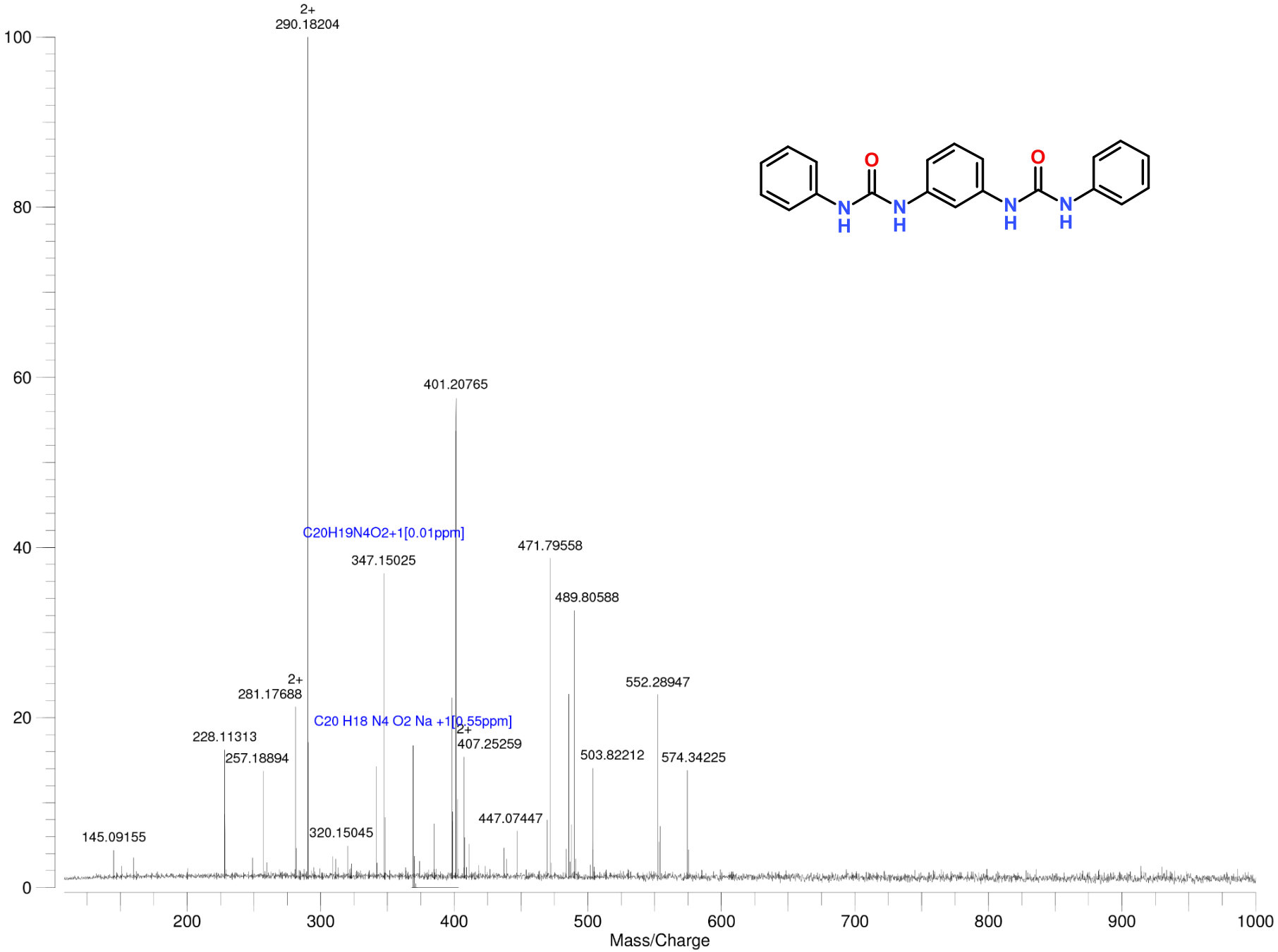


^{13}C NMR spectrum of compound U11

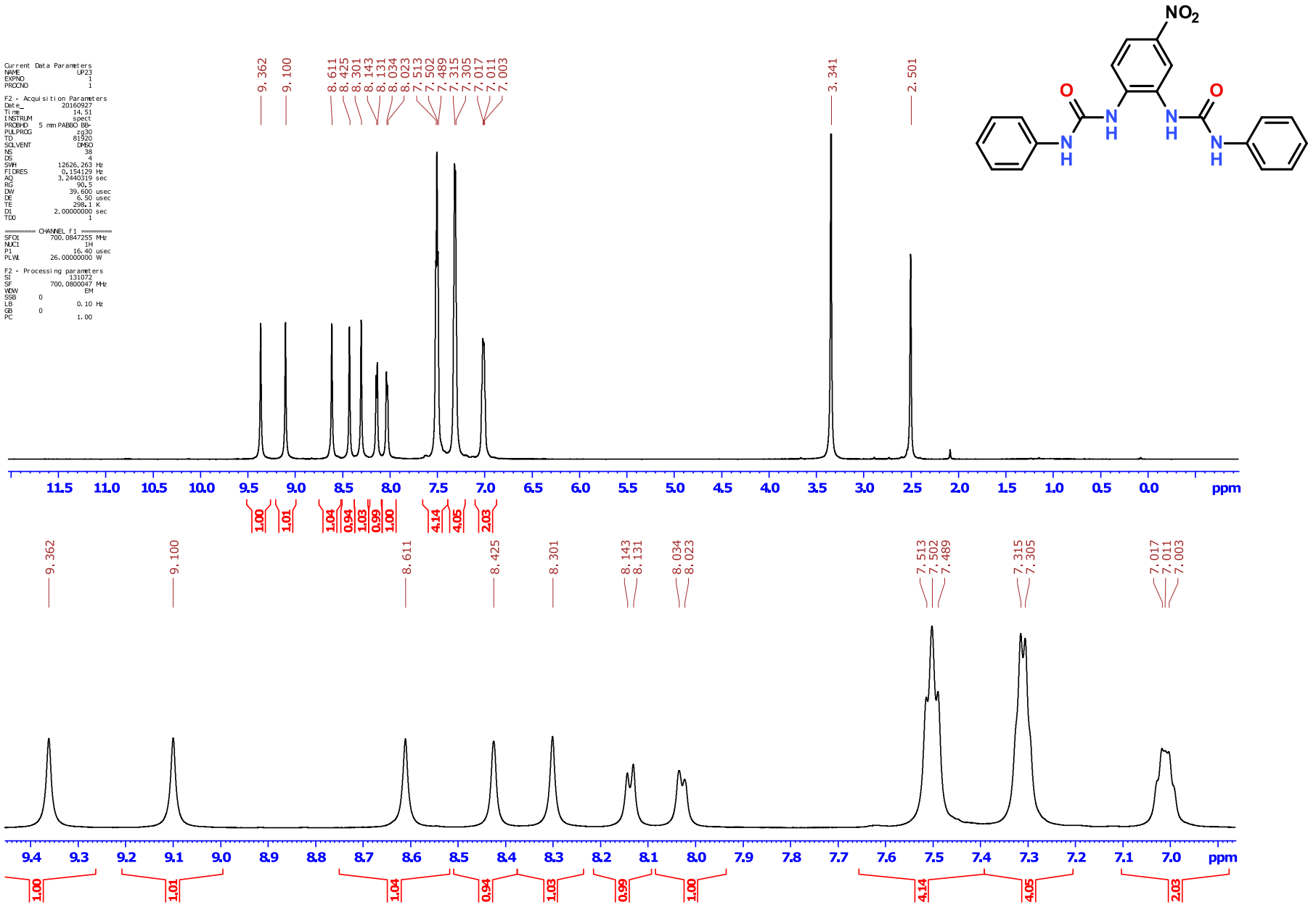




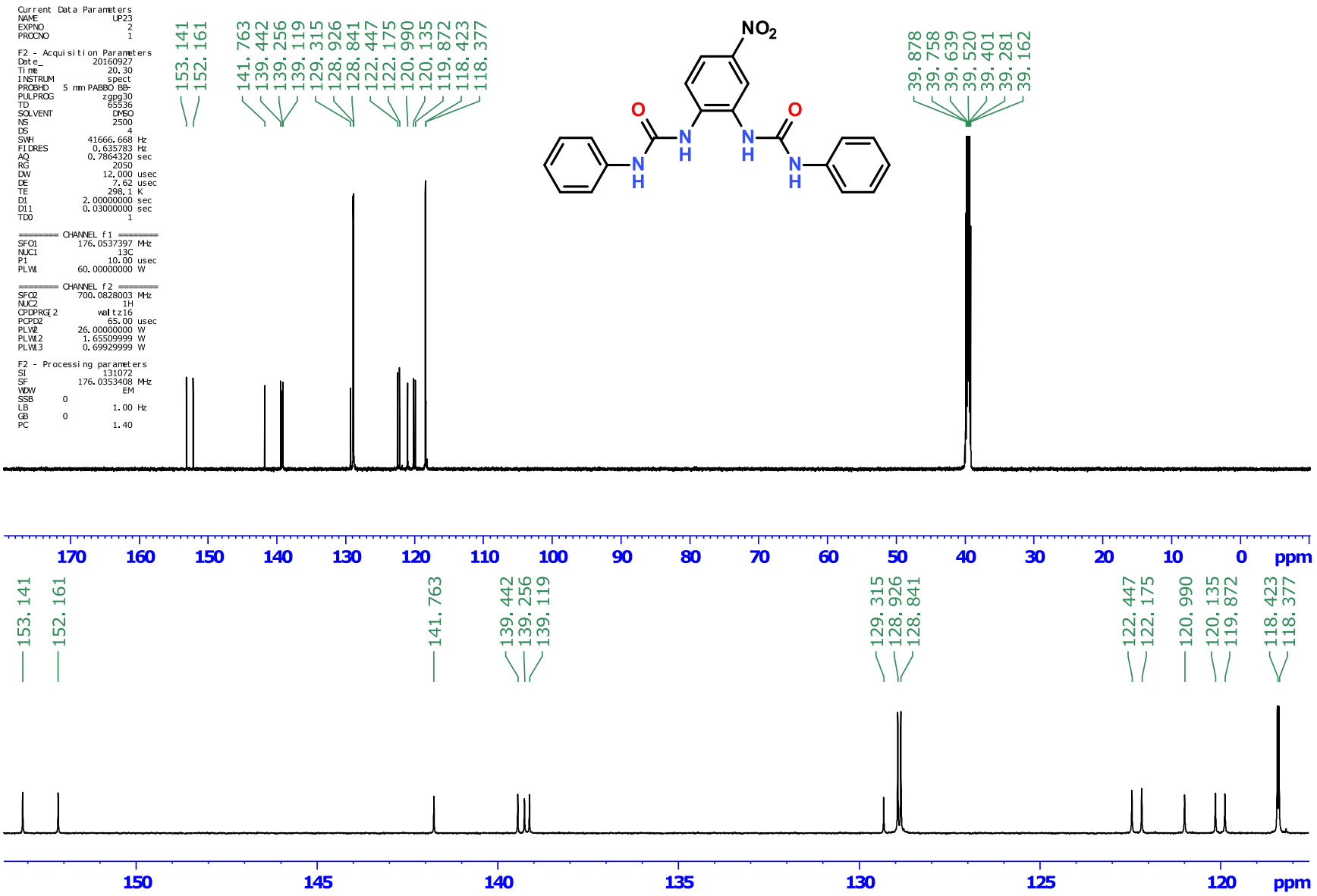
HRMS spectrum of compound U11



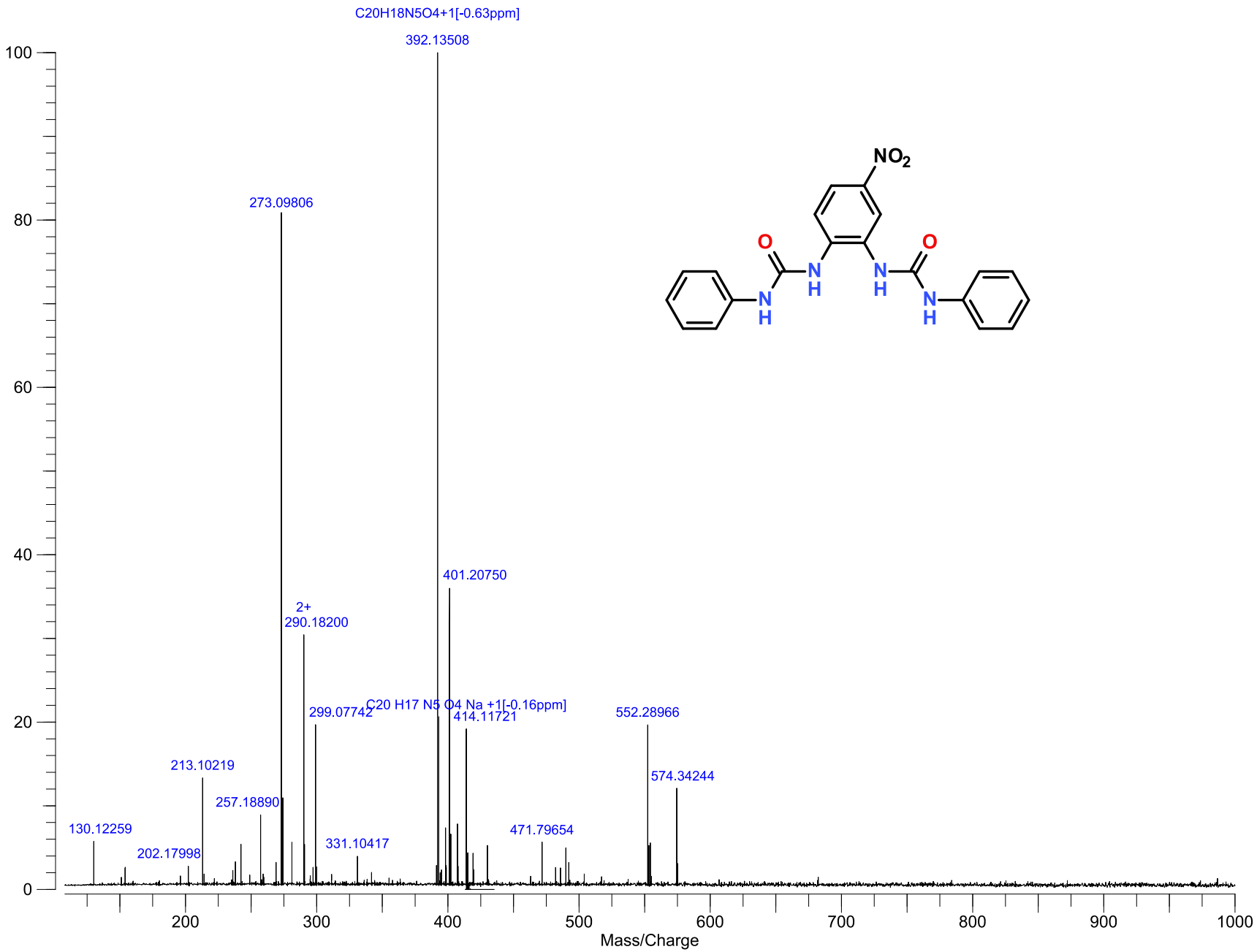
^{1}H NMR spectrum of compound U14



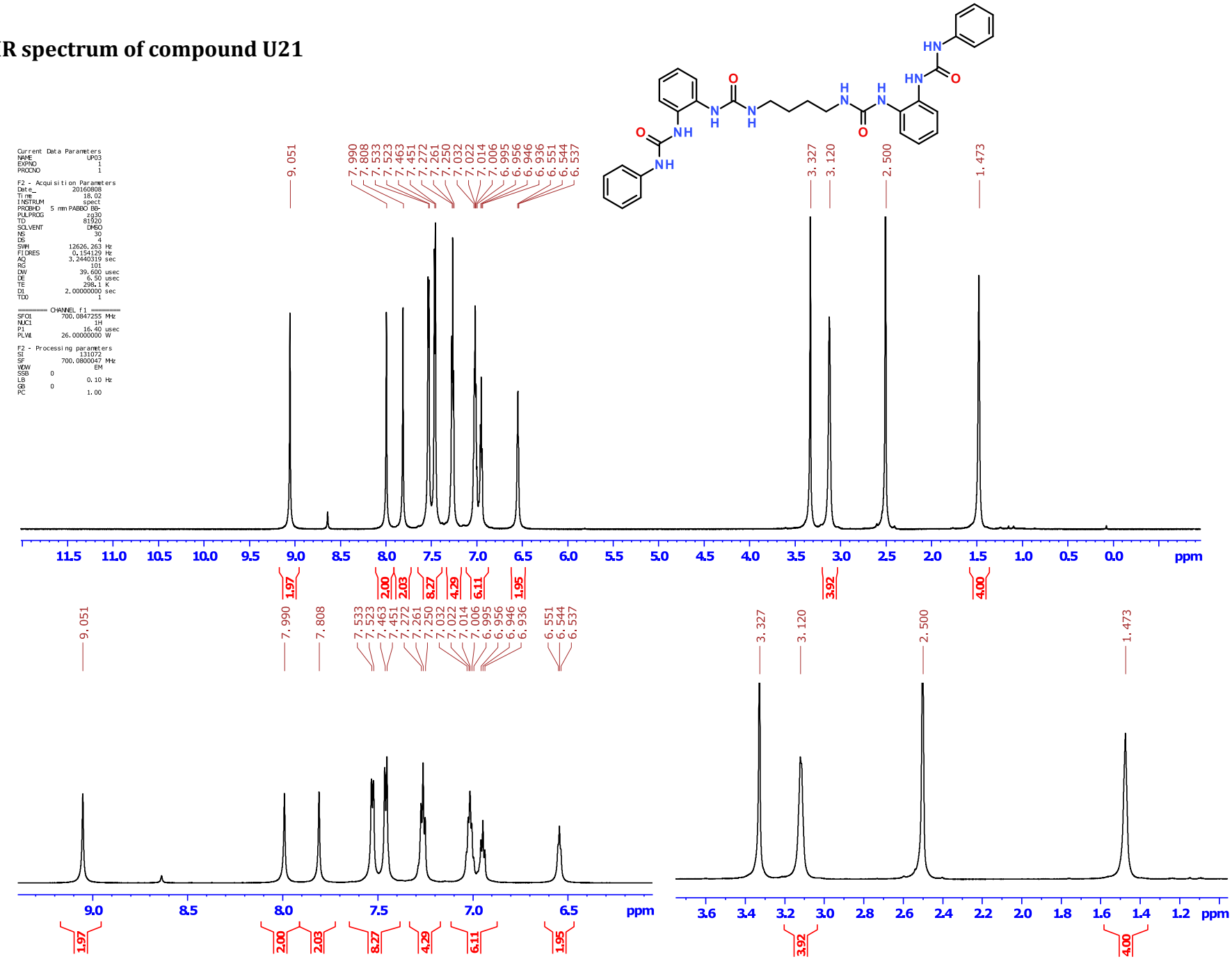
^{13}C NMR spectrum of compound U14



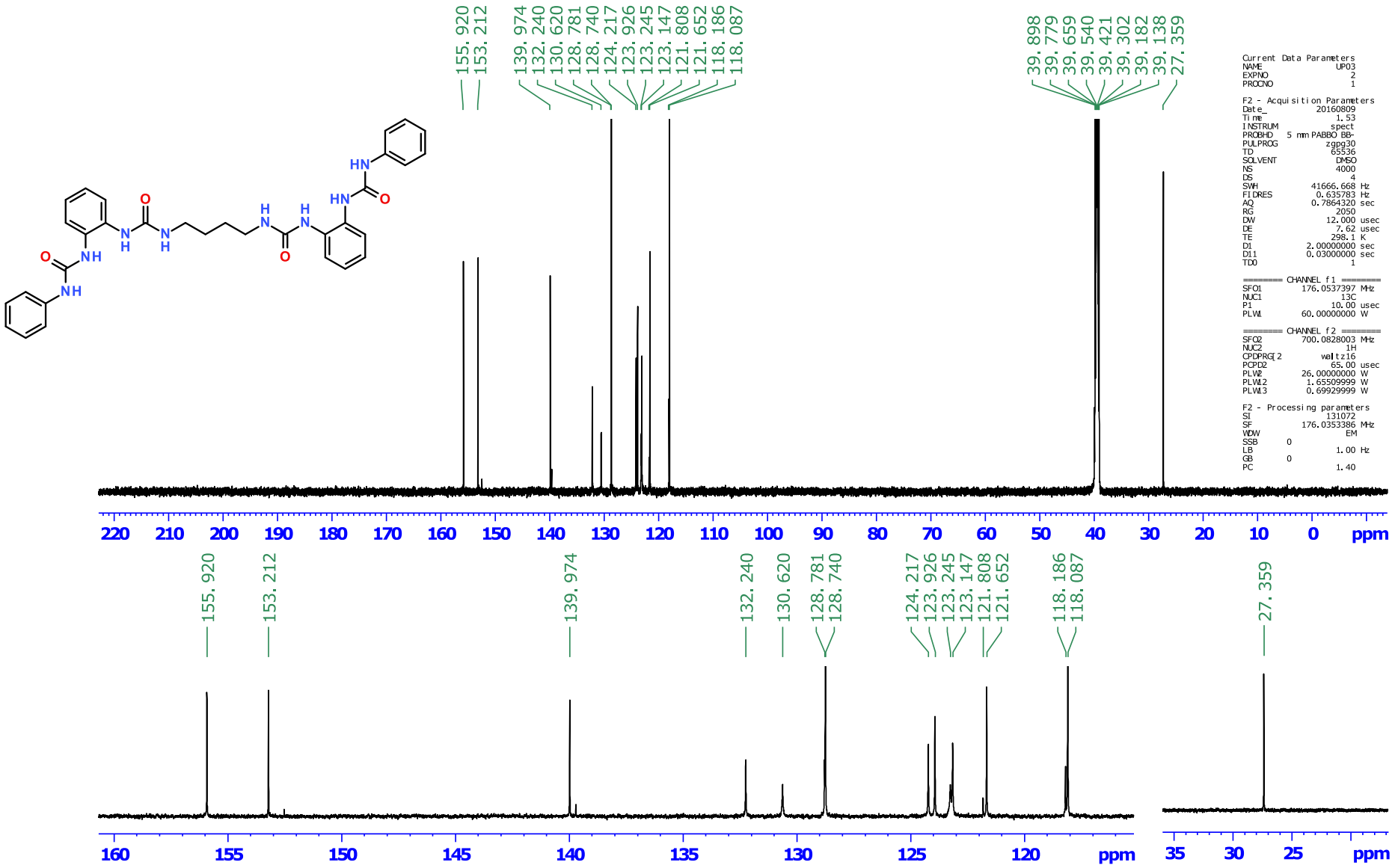
HRMS spectrum of compound U14



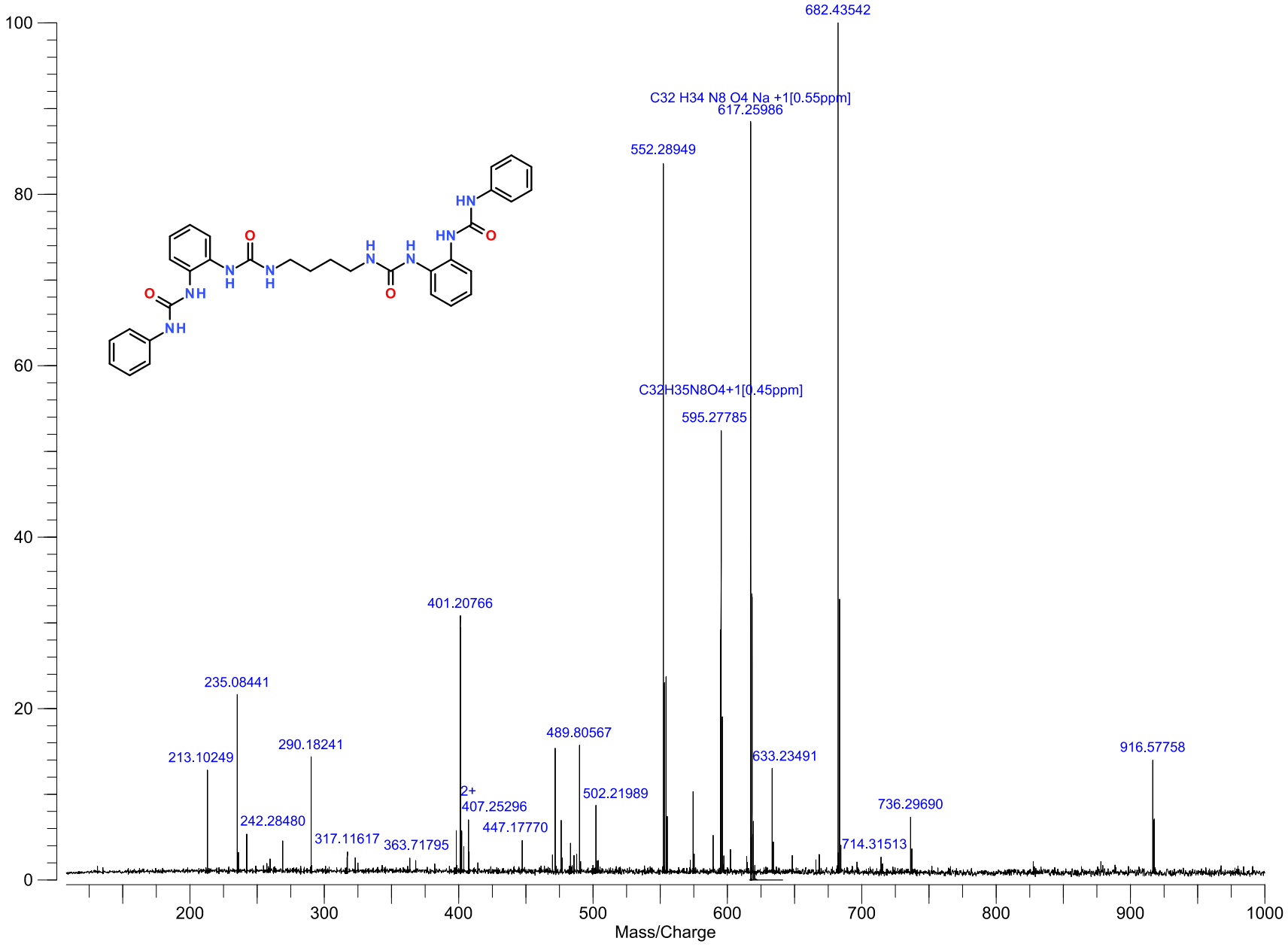
^{1}H NMR spectrum of compound U21



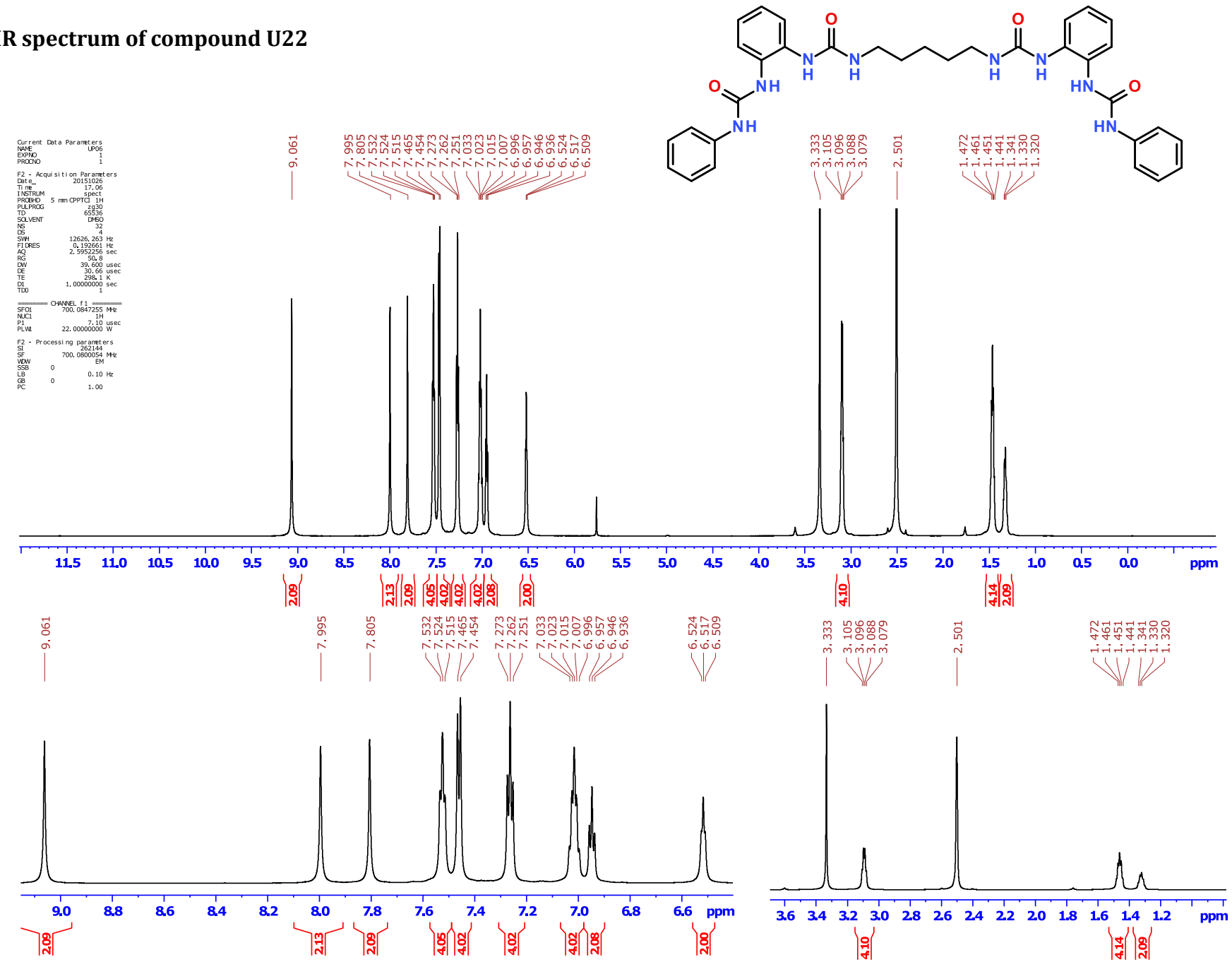
^{13}C NMR spectrum of compound U21



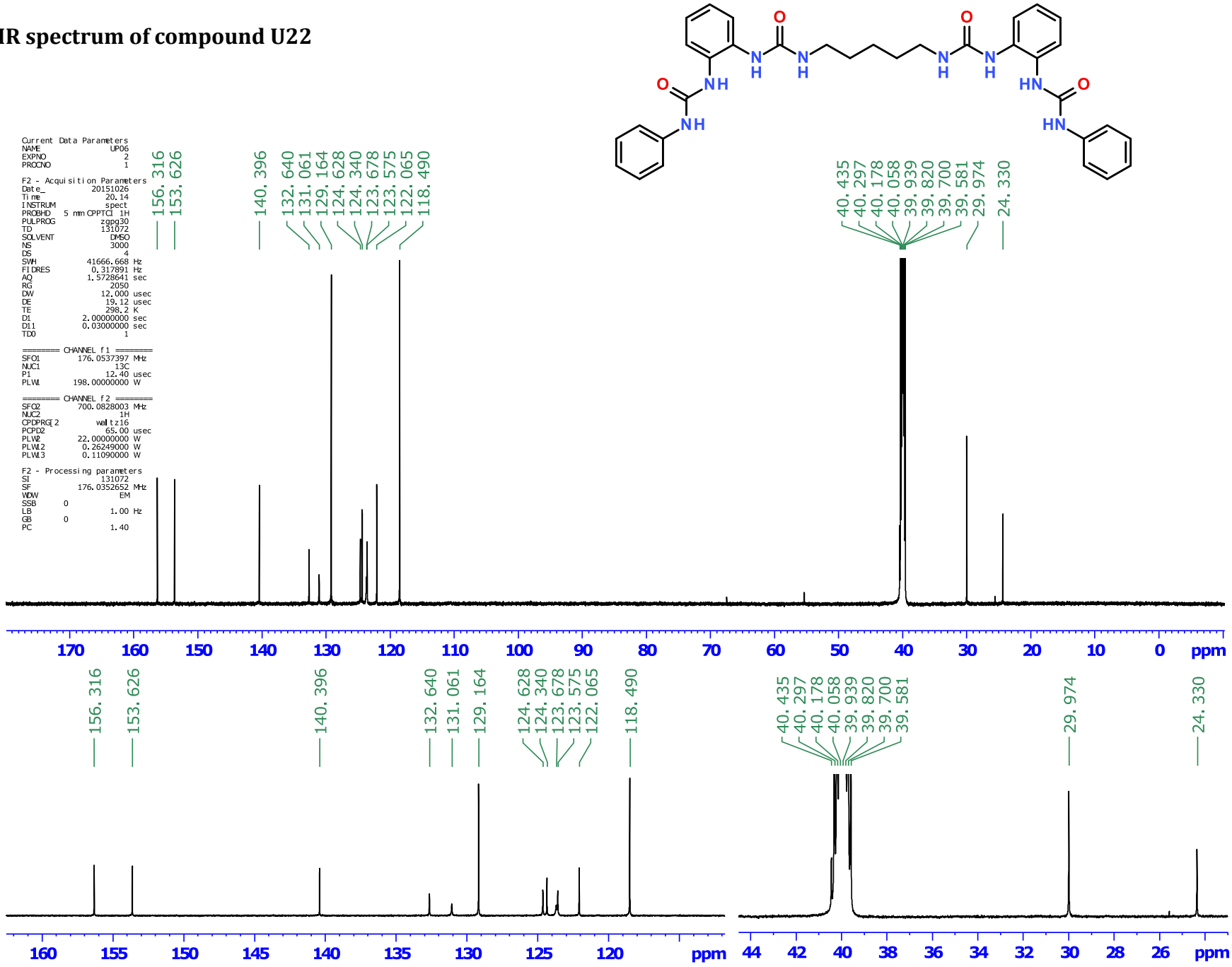
HRMS spectrum of compound U21



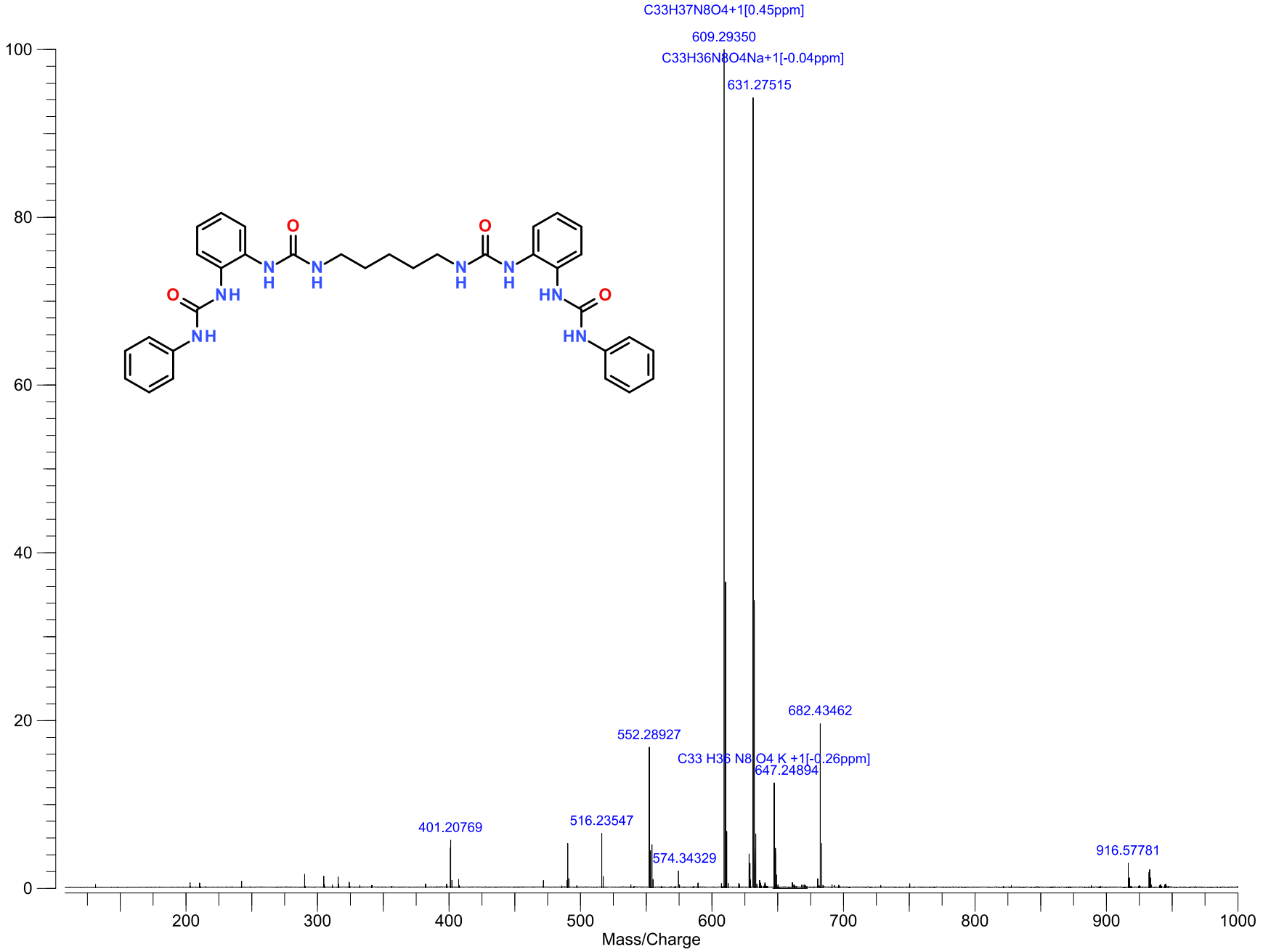
^{1}H NMR spectrum of compound U22



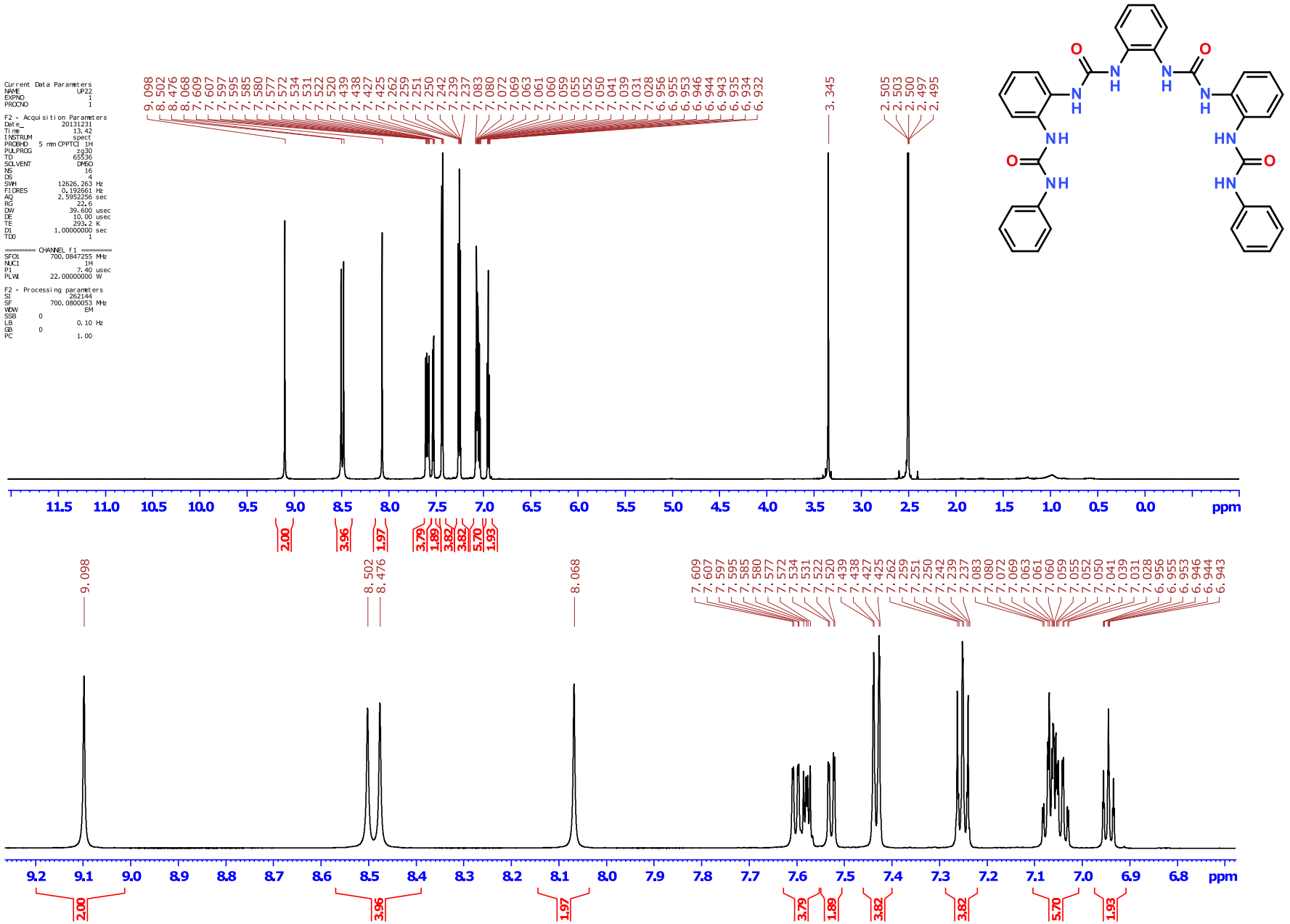
^{13}C NMR spectrum of compound U22



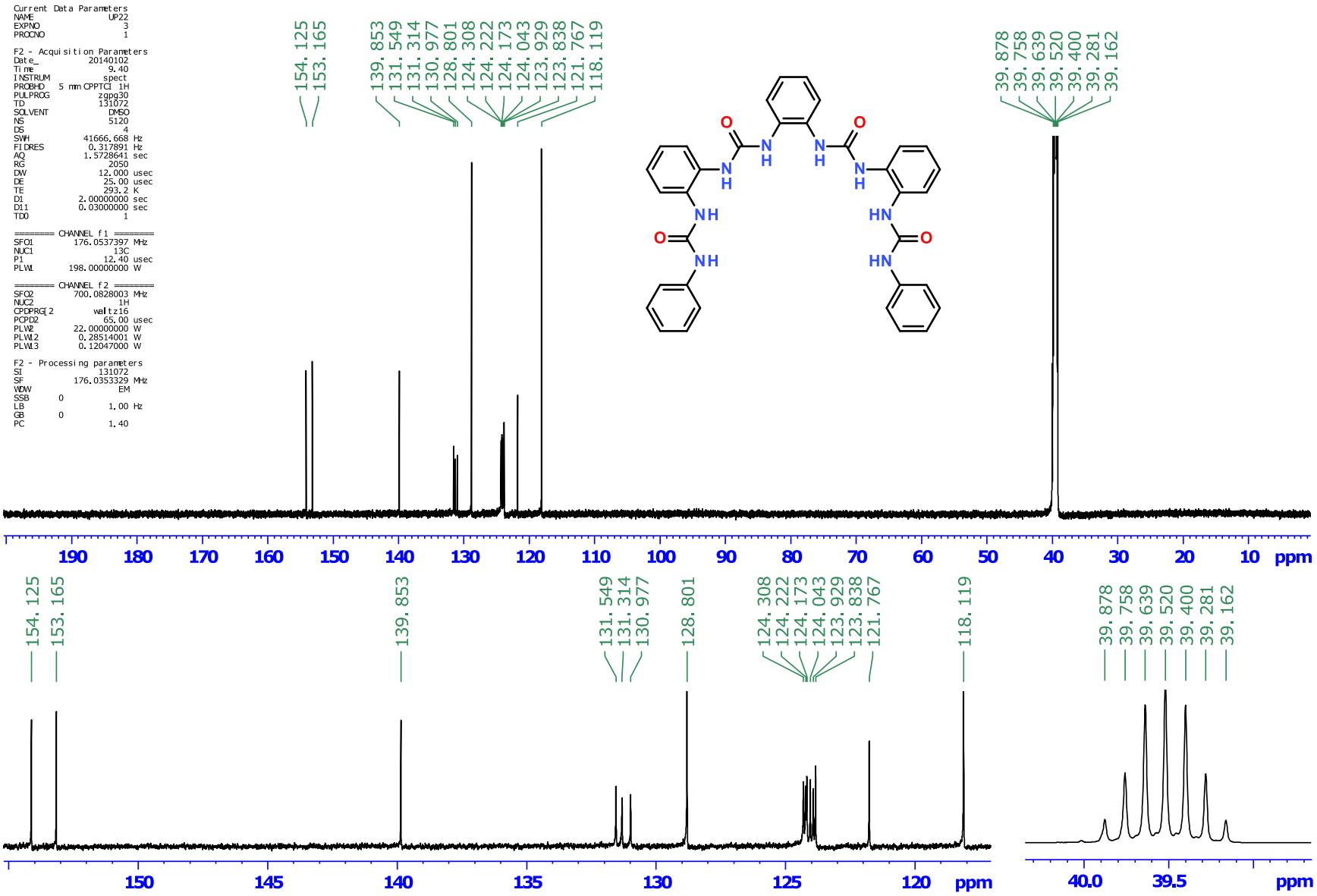
HRMS spectrum of compound U22



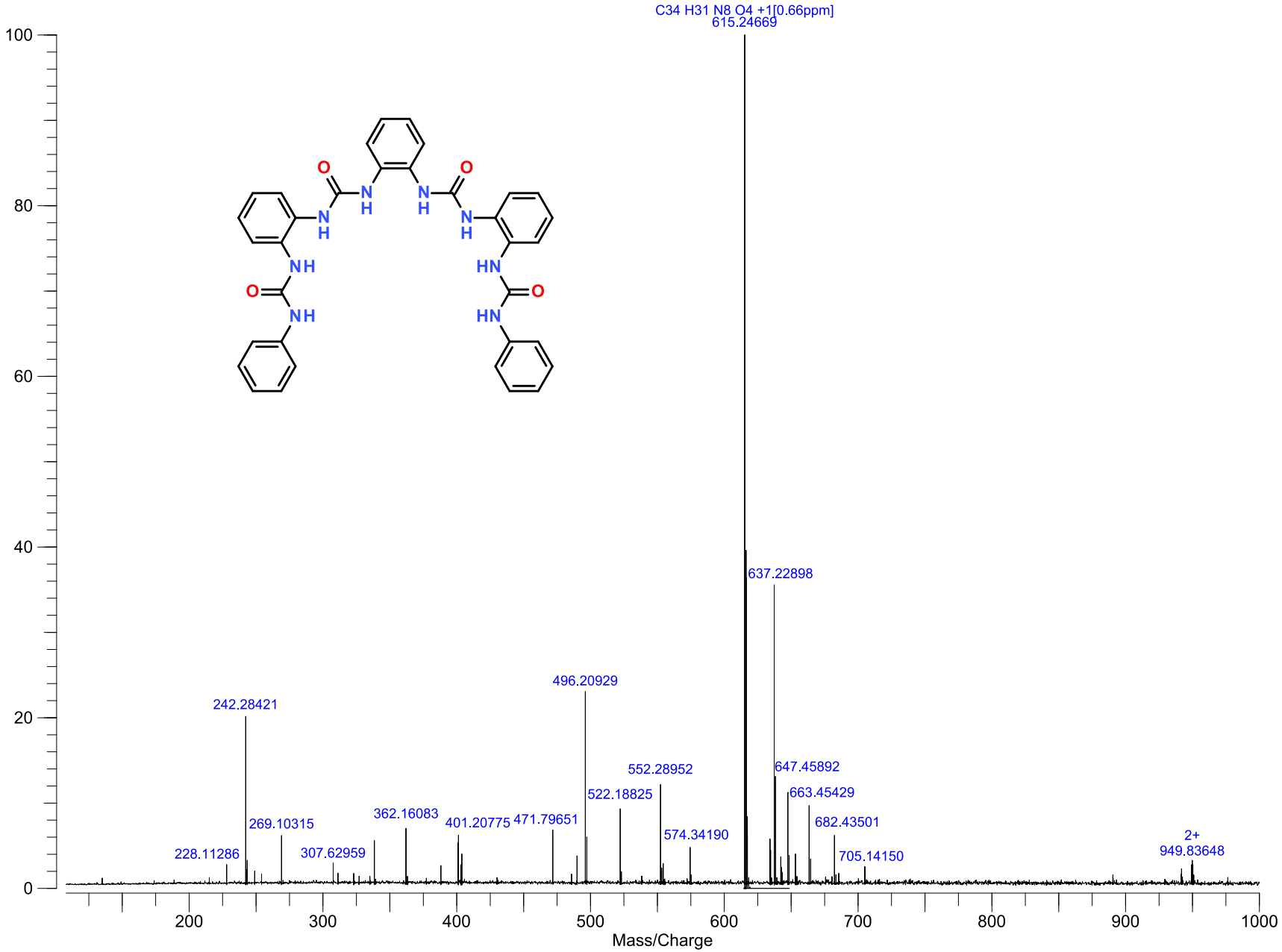
^{1}H NMR spectrum of compound U23



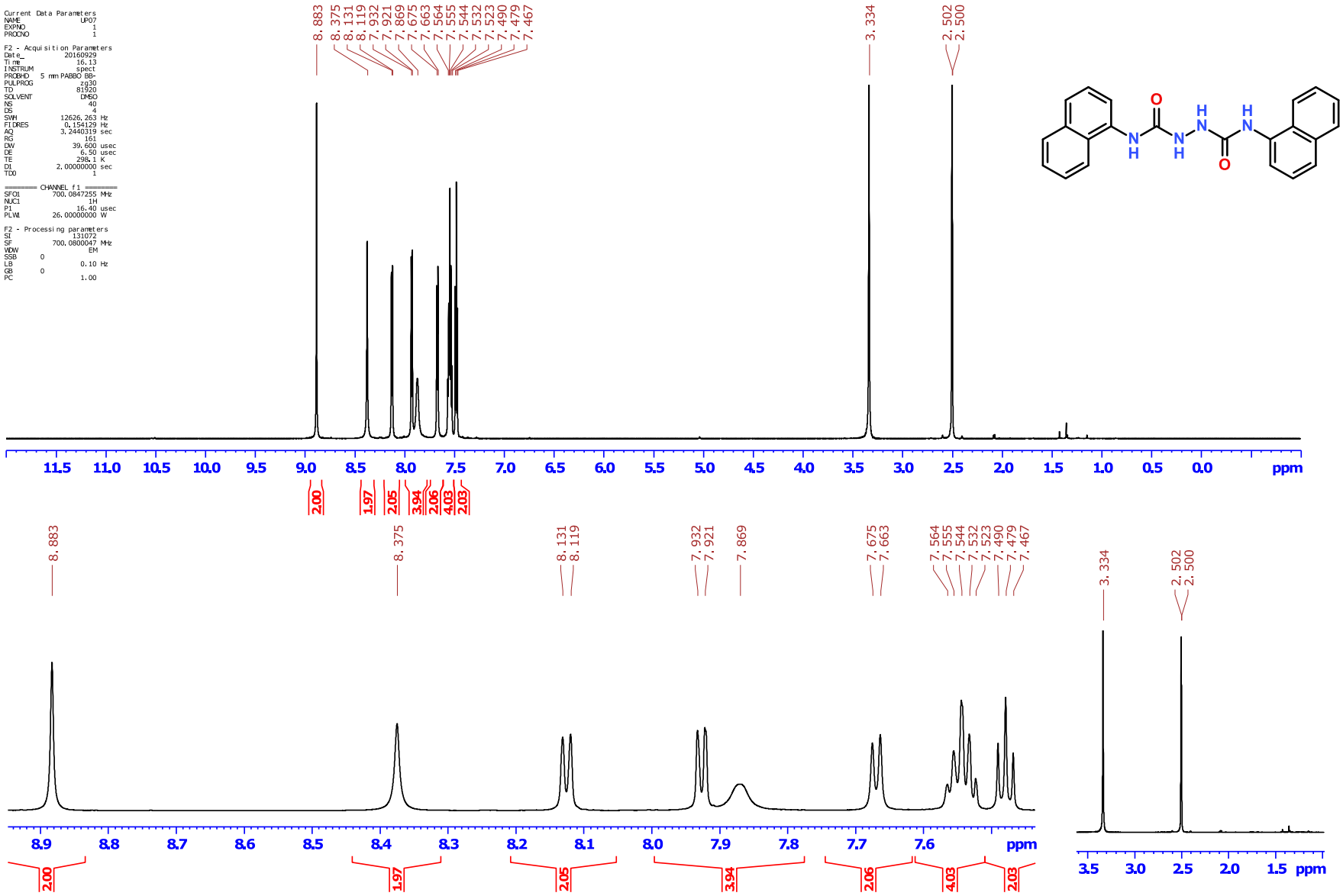
^{13}C NMR spectrum of compound U23



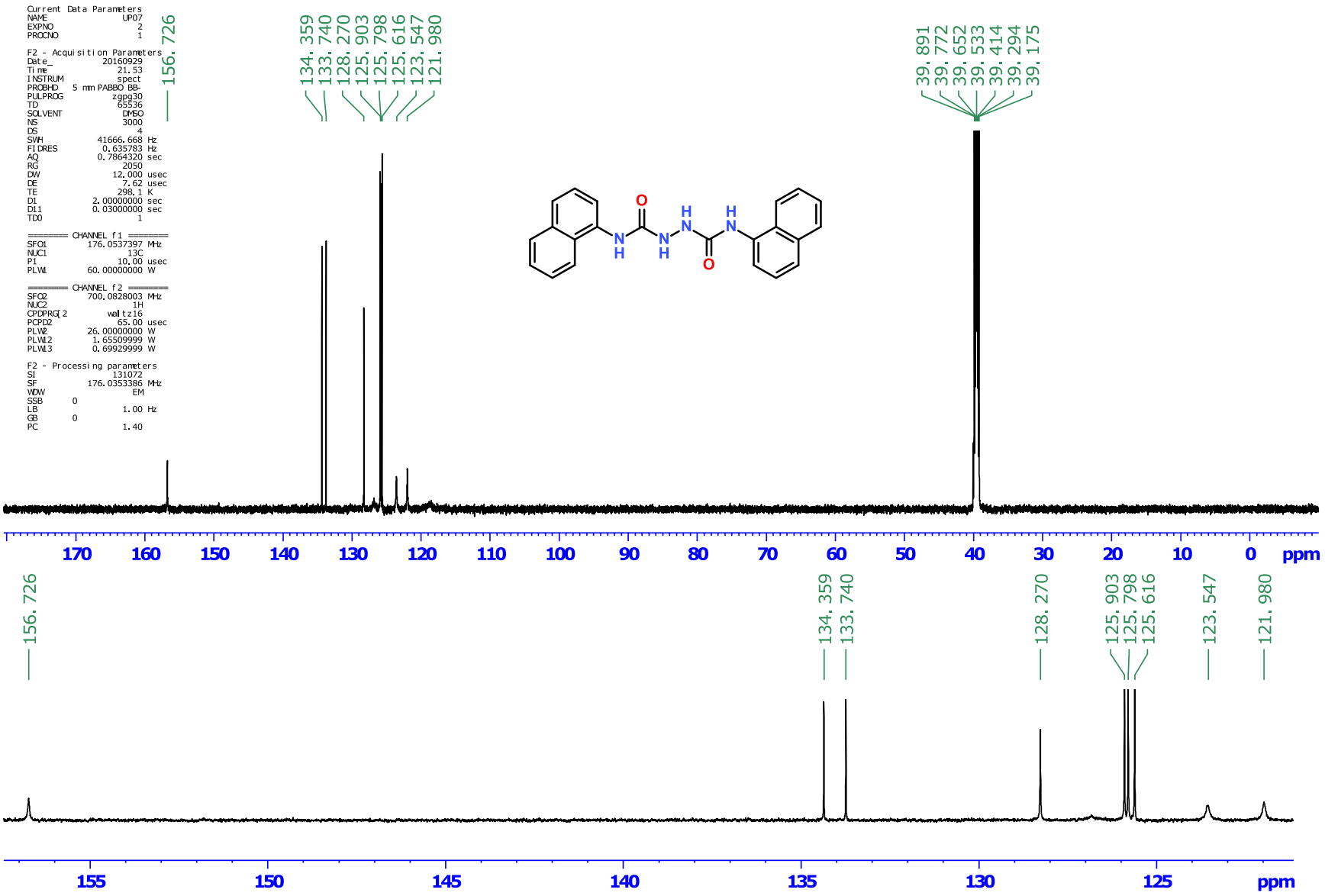
HRMS spectrum of compound U23



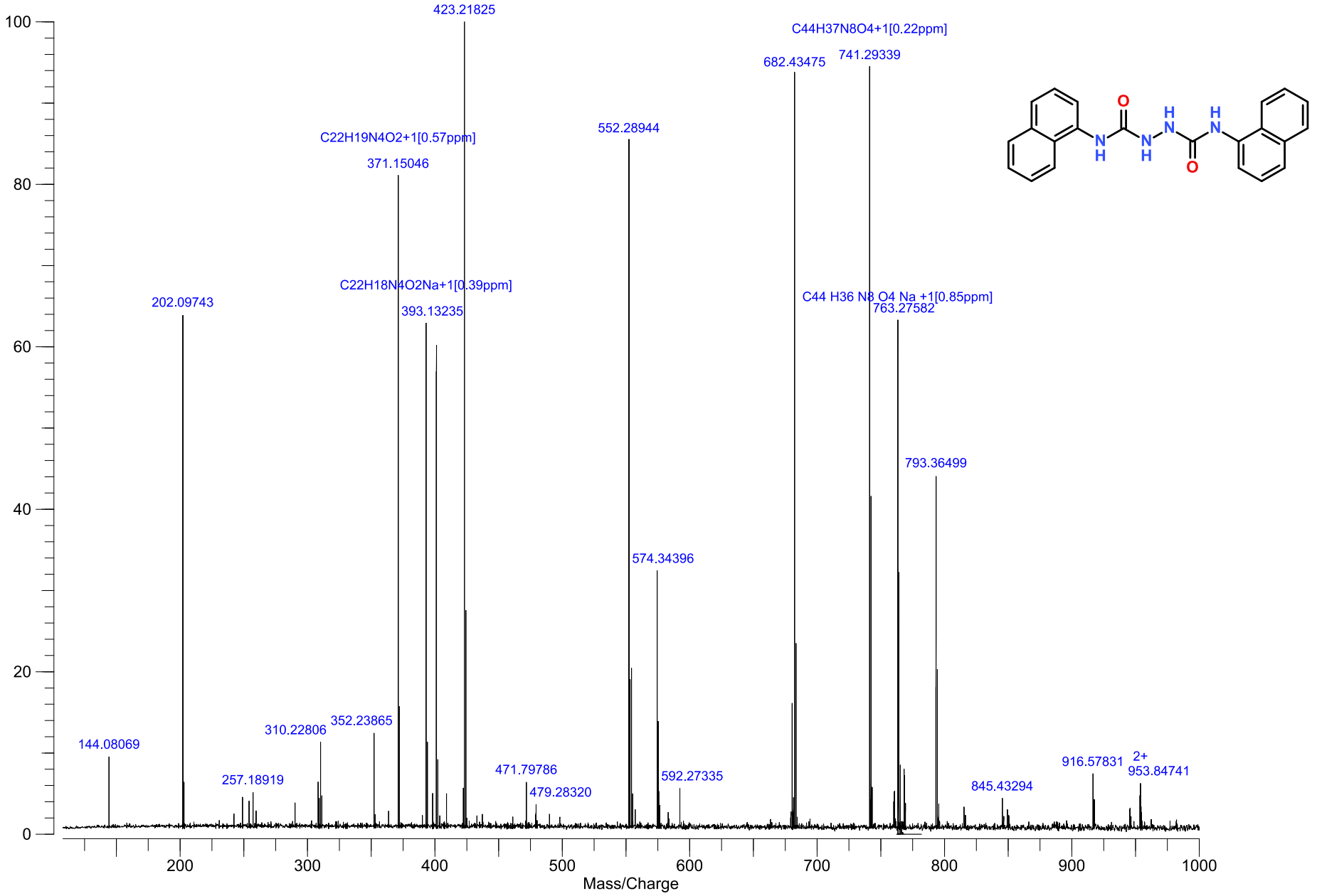
^{1}H NMR spectrum of compound HZ01



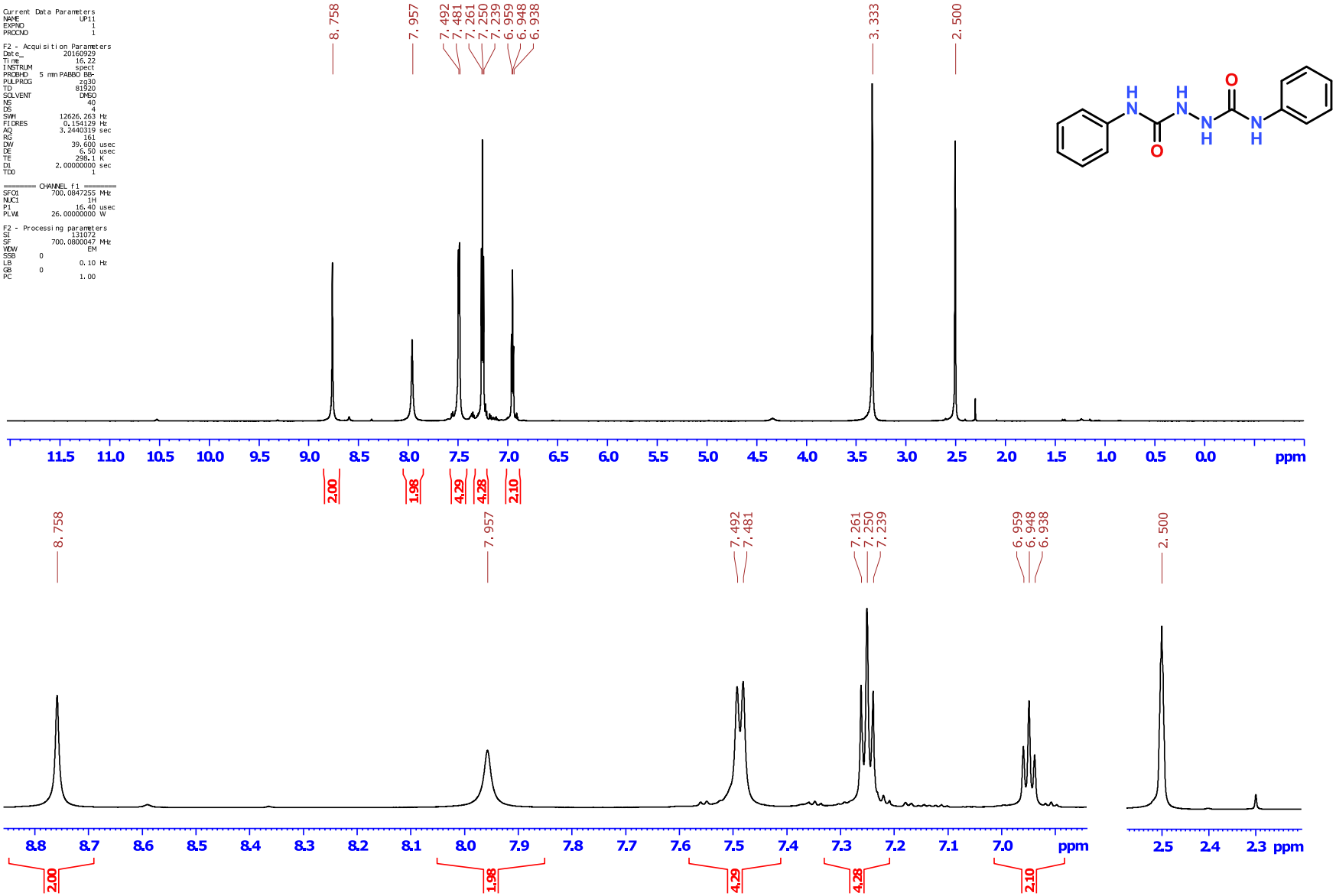
^{13}C NMR spectrum of compound HZ01



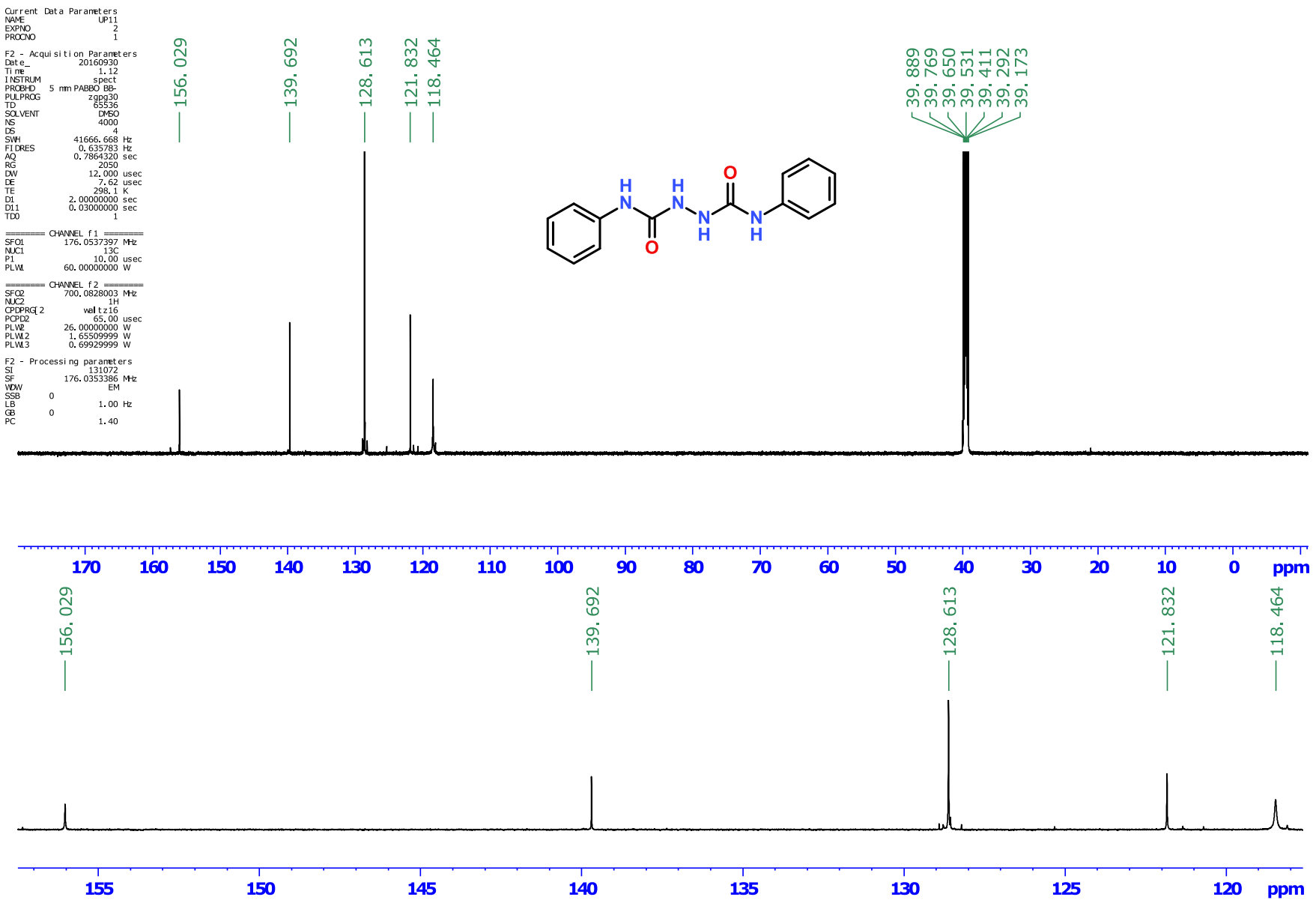
HRMS spectrum of compound HZ01



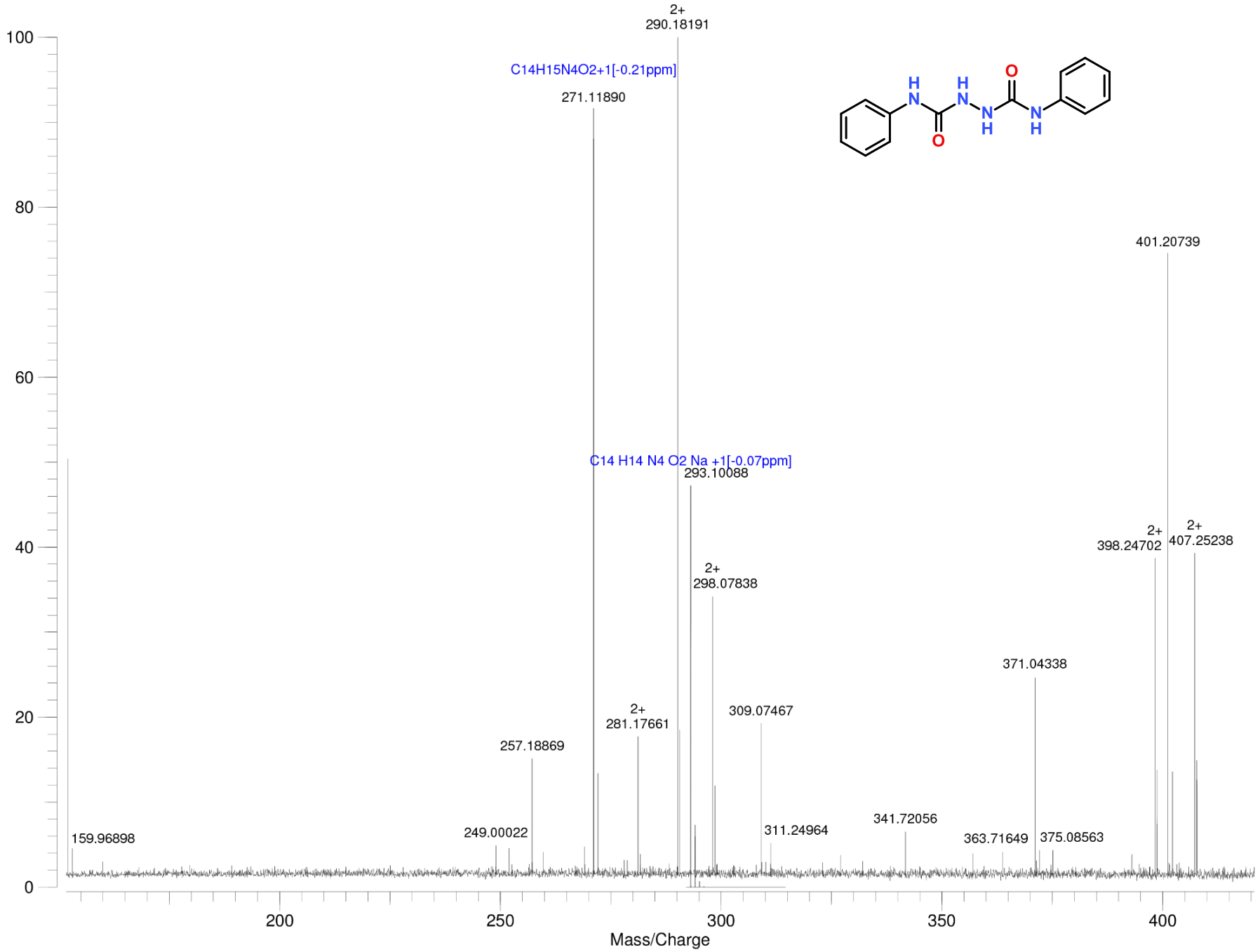
^{1}H NMR spectrum of compound HZ02



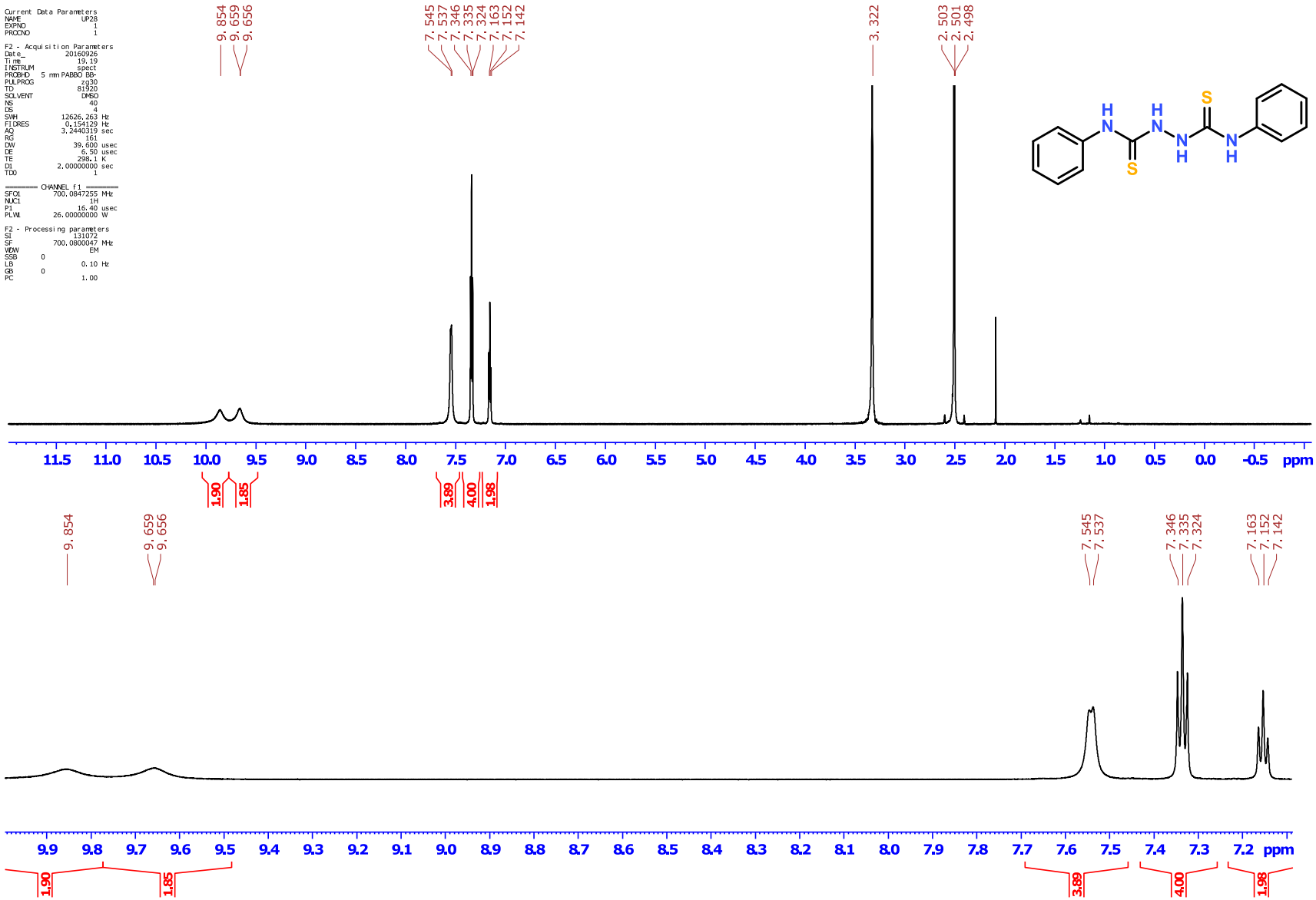
^{13}C NMR spectrum of compound HZ02



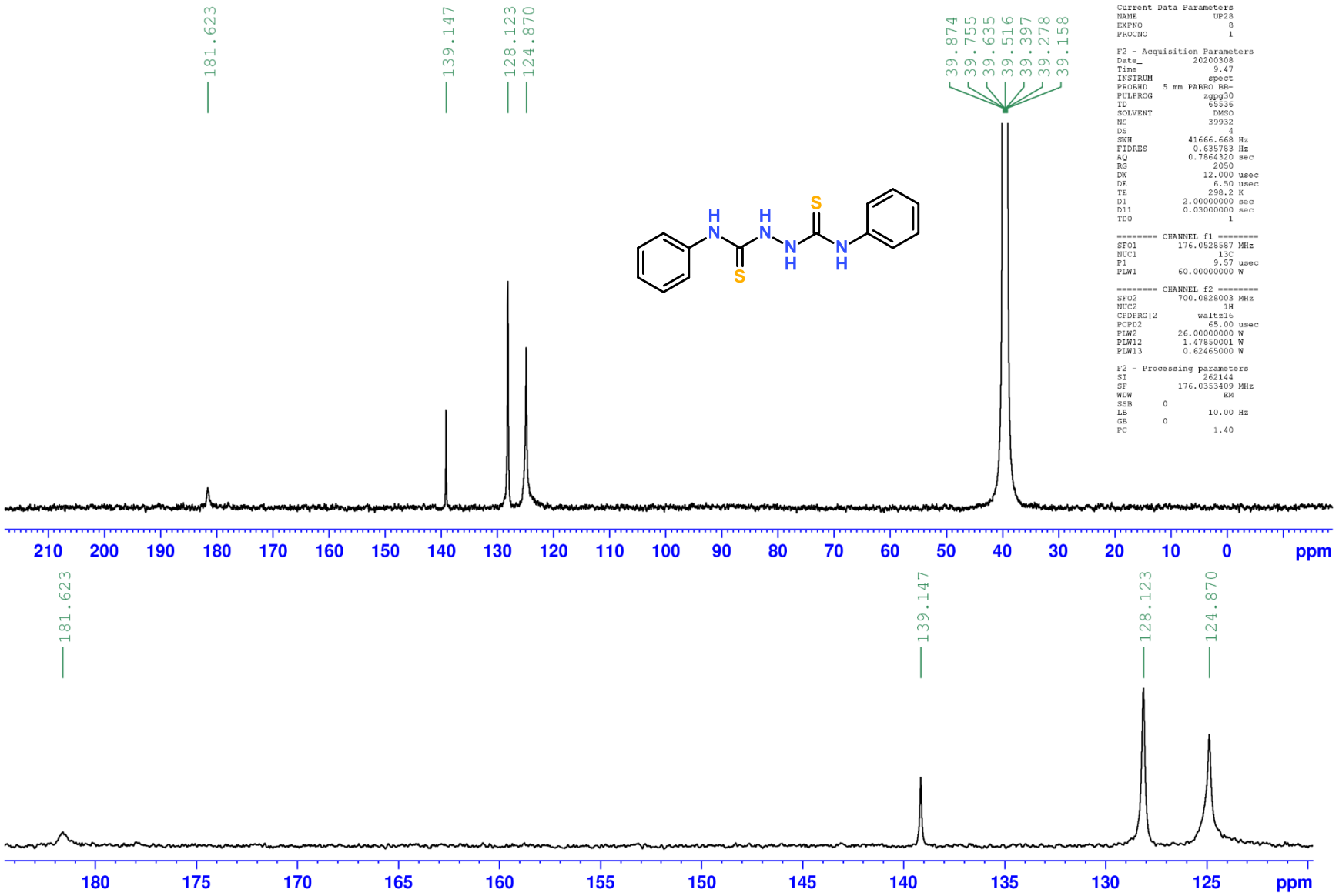
HRMS spectrum of compound HZ02



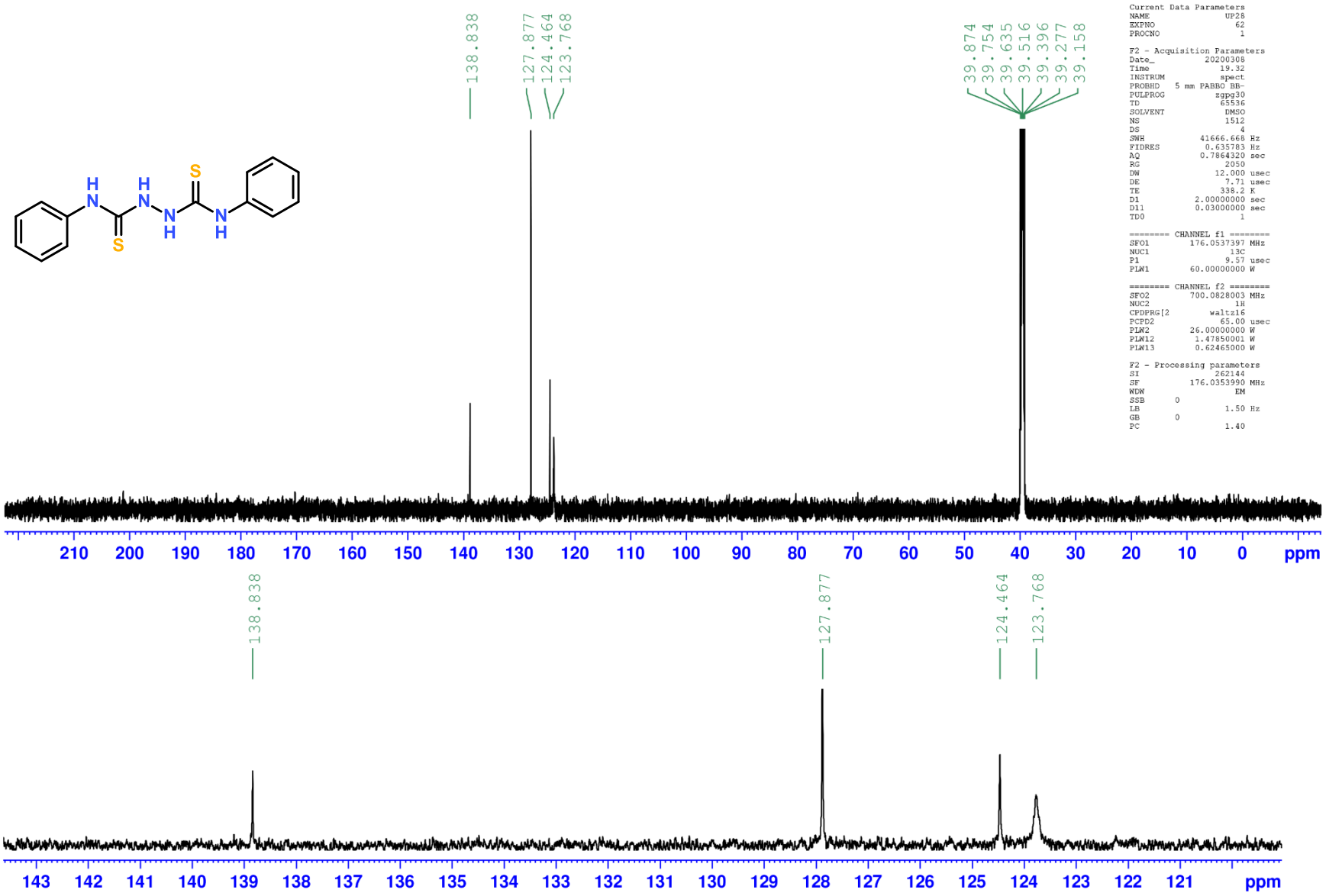
^{1}H NMR spectrum of compound HZ03



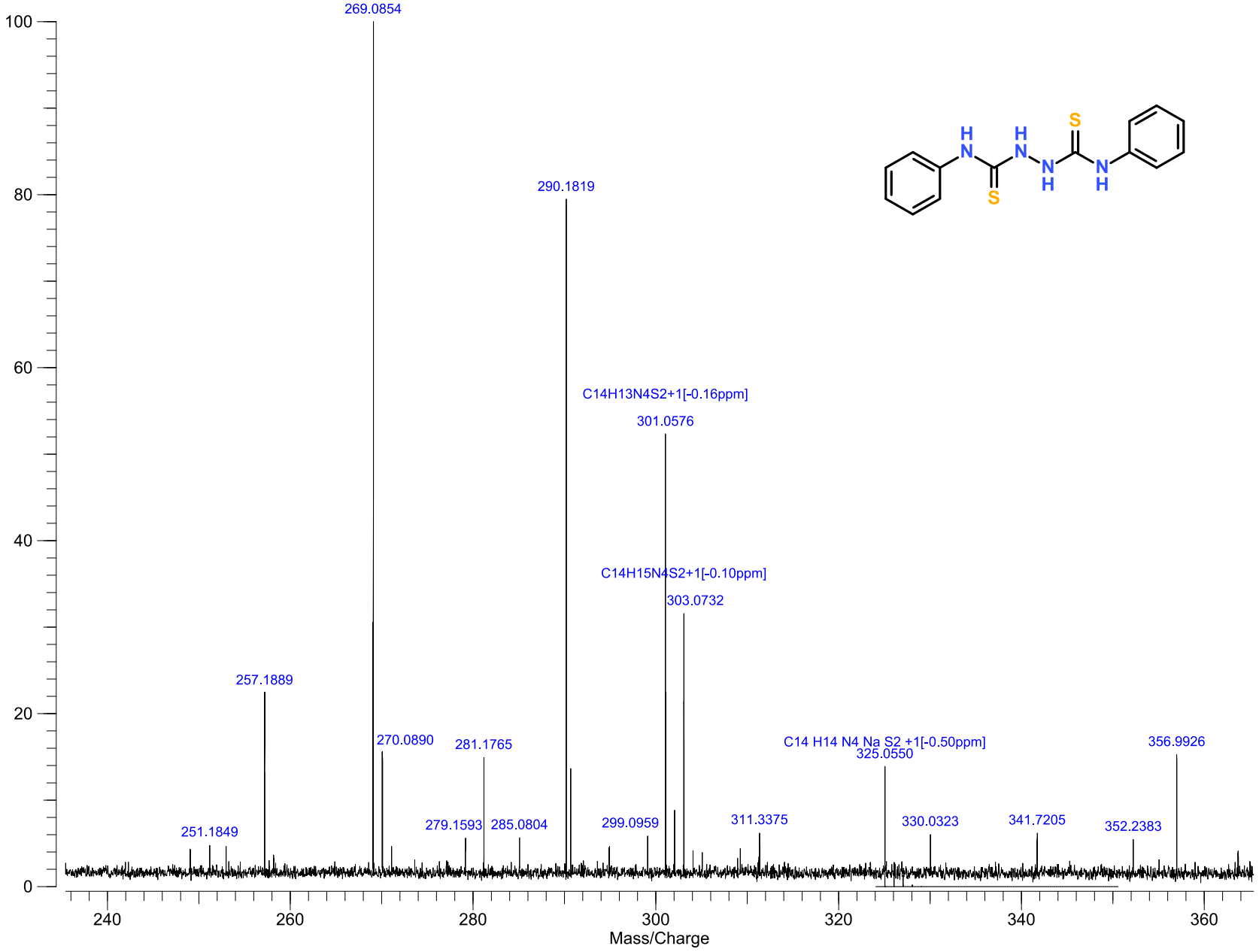
^{13}C NMR (+25 °C) spectrum of compound HZ03



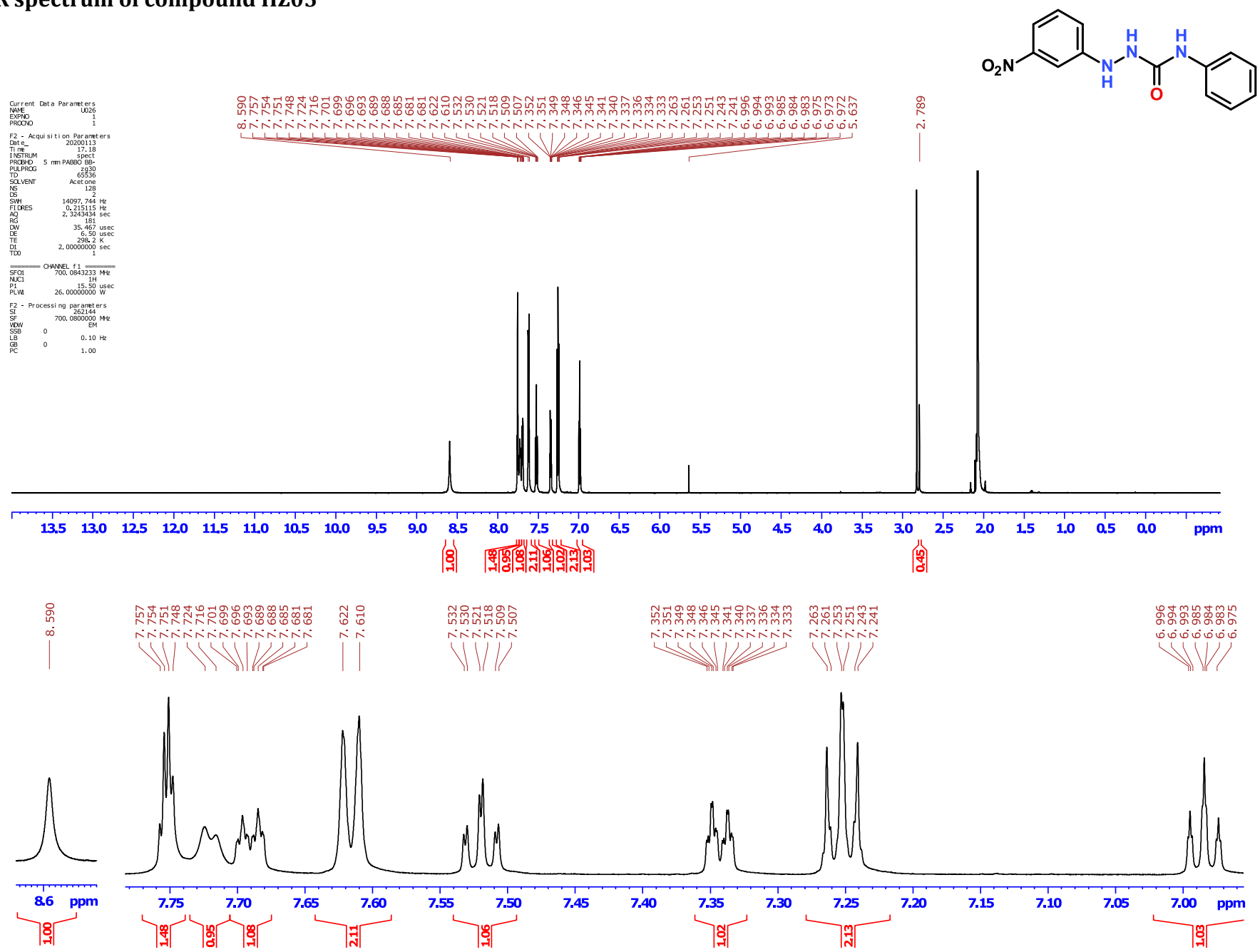
^{13}C NMR (+65 °C) spectrum of compound HZ03



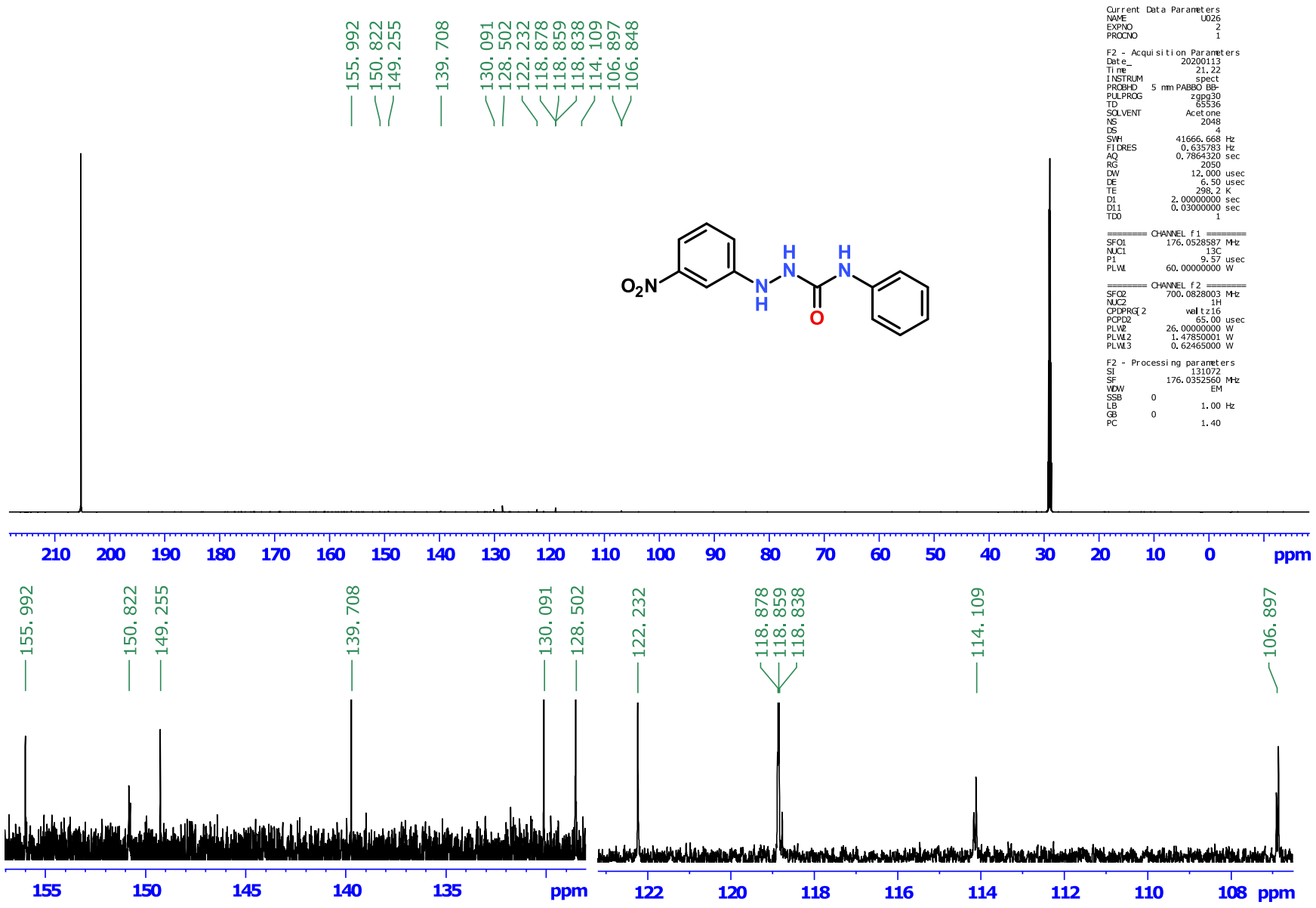
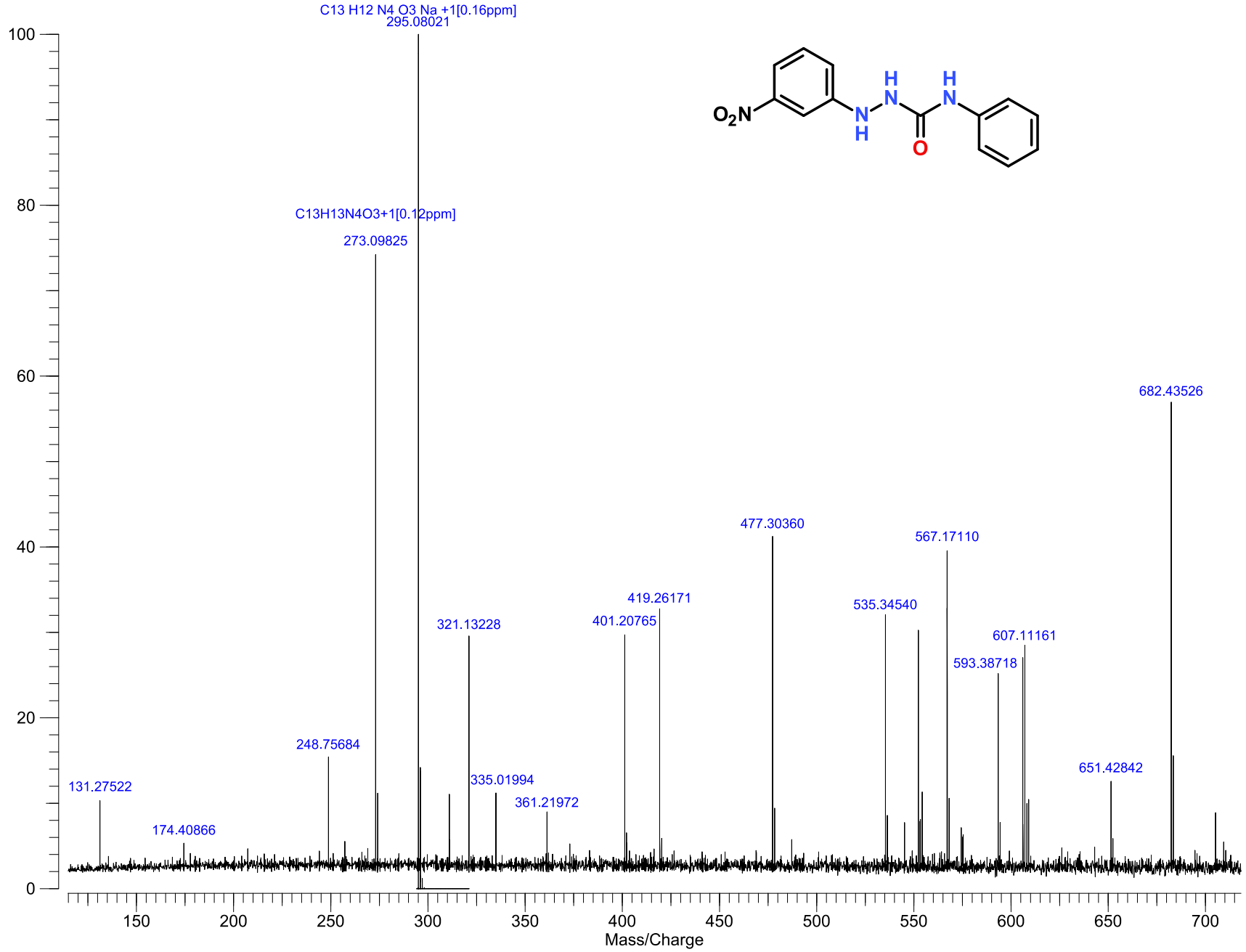
HRMS spectrum of compound HZ03



^{1}H NMR spectrum of compound HZ05



^{13}C NMR spectrum of compound HZ05



HRMS spectrum of compound HZ05