ELECTRONIC SUPPLEMENTARY MATERIALS

N-Substituted tetrahydropentaazadibenzocycloheptafluorenes – a new type of condensed polyazapolycyclic system

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Leonard M. Khalilov, Askhat G. Ibragimov

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11b,11c-Dihydro-6*H*,12*H*-4b,5a,10b,11a-tetraazadibenzo[*a,h*]cyclopenta[*def*]fluorene (**2**)

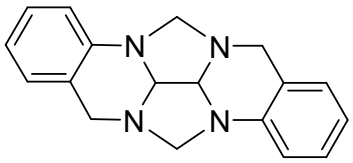
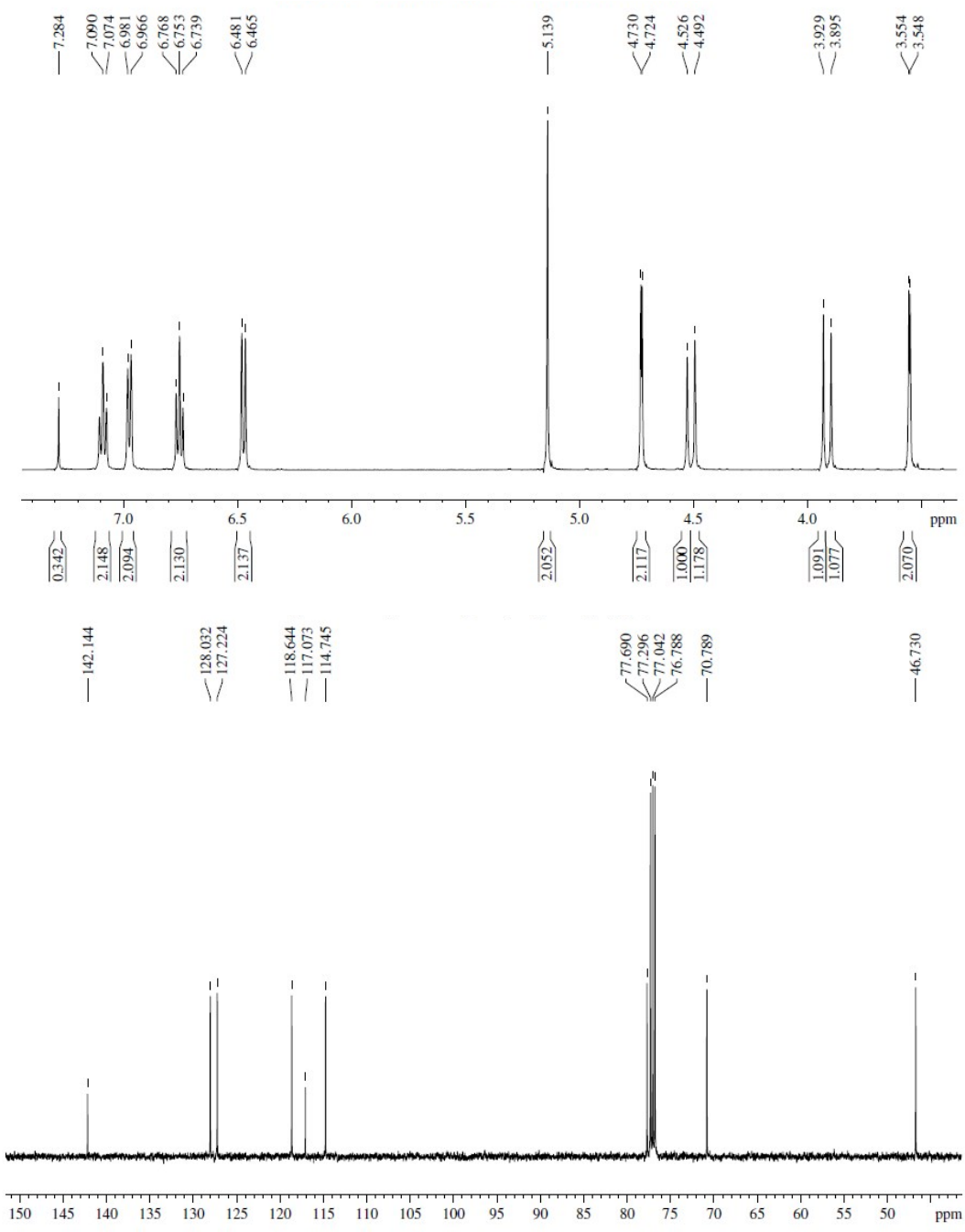
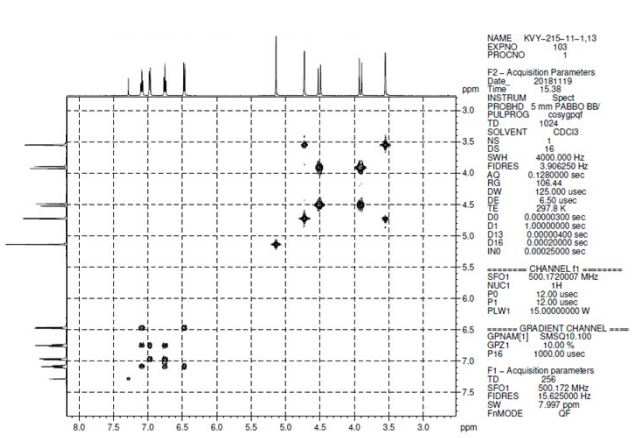


Figure 1. NMR and MS spectra of compound **2**.

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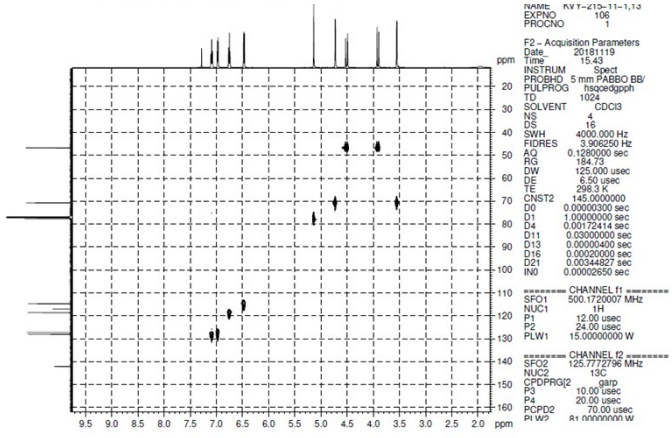
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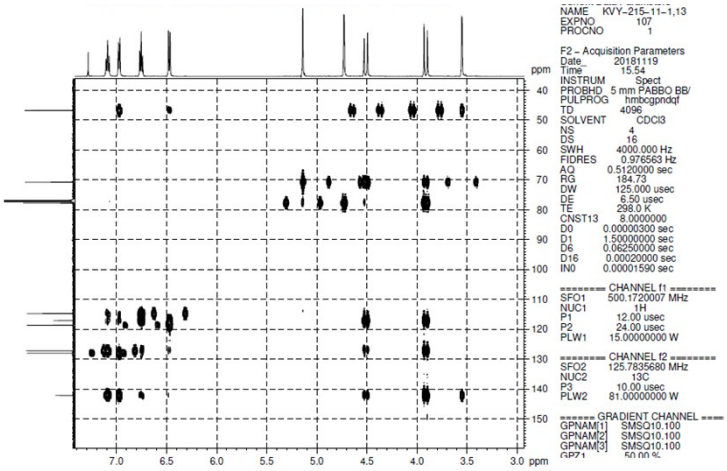
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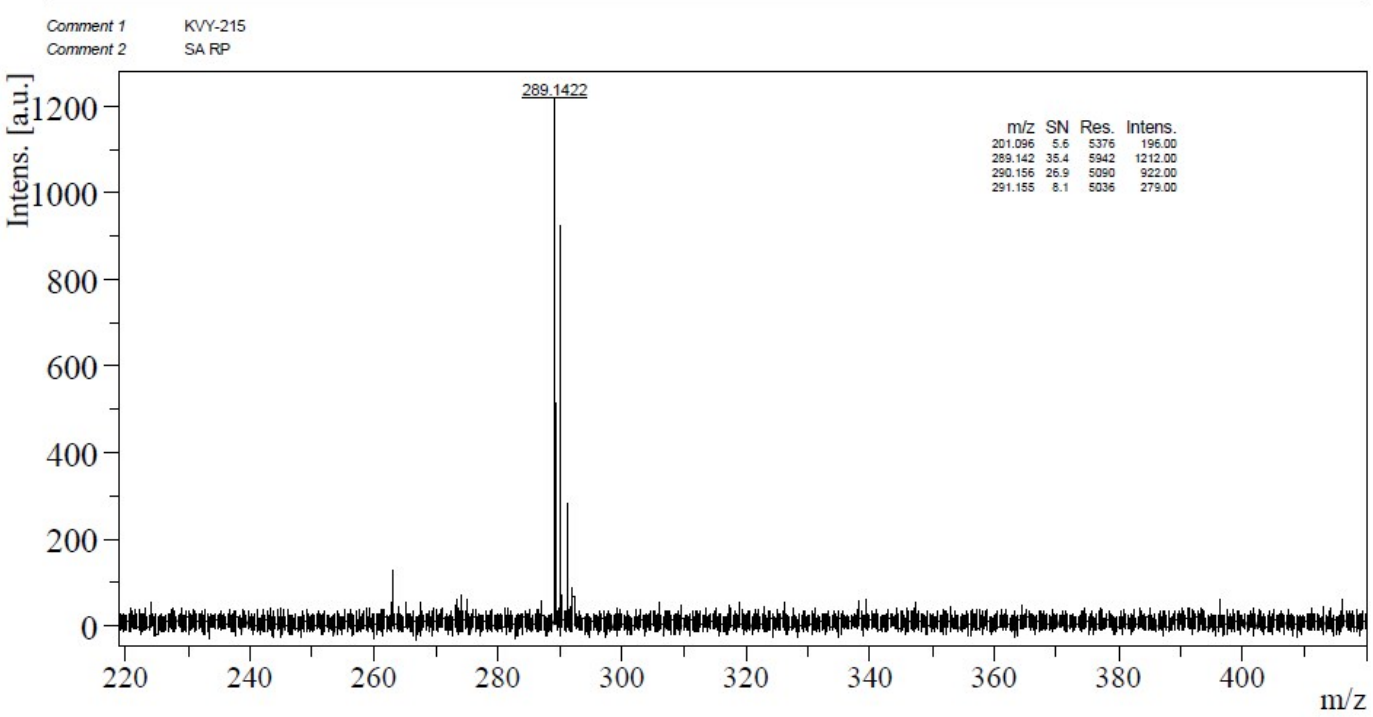
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Intens. [a.u.]
m/z

12-Cyclopropyl-12,13,13b,13c-tetrahydro-6*H*,11*H*,14*H*-4b,5a,10b,12,13a-pentaazadibenzo[*a,h*]cyclohepta[1,2,3,4-*def*]fluorene (**3**)

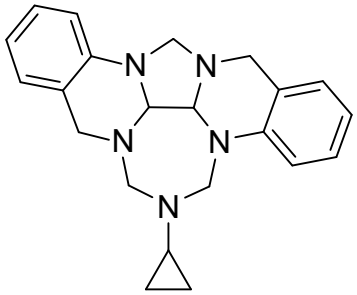
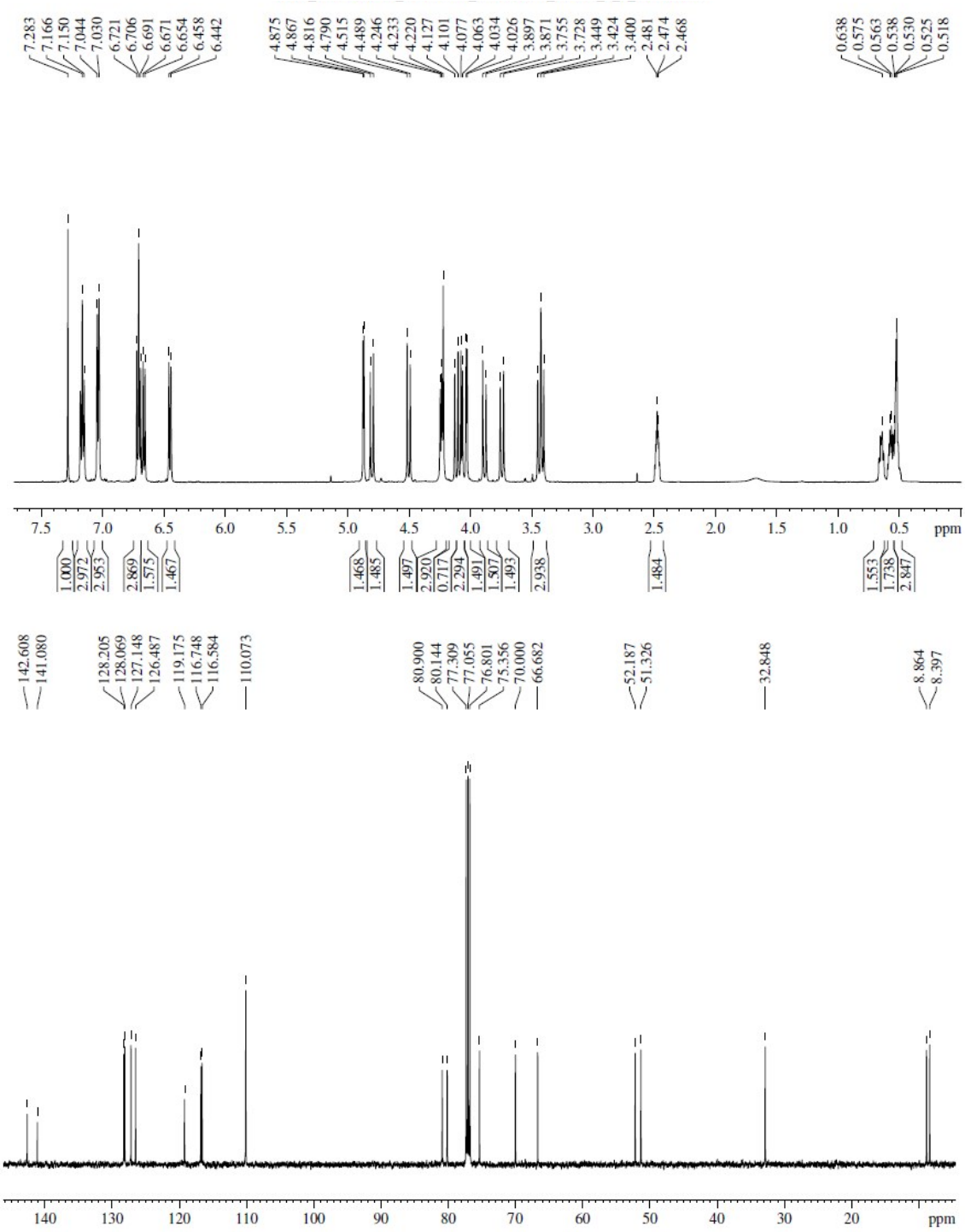
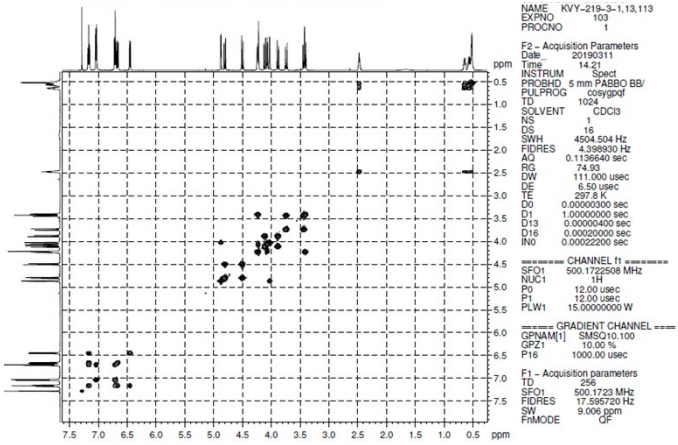
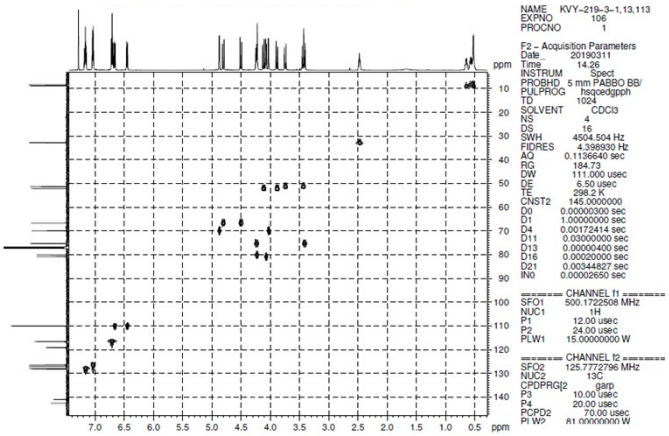
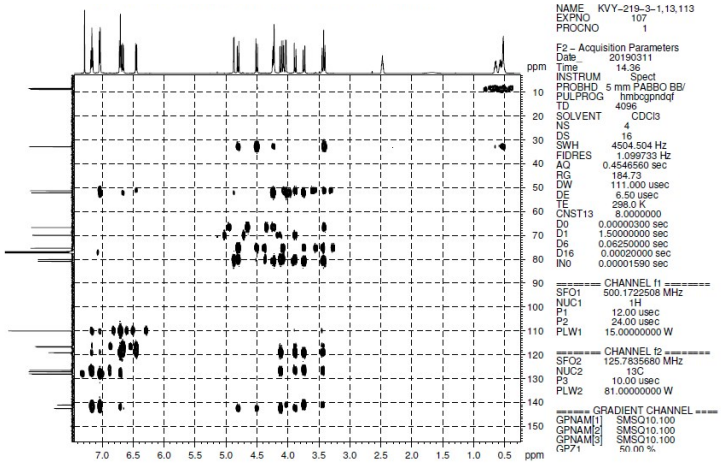


Figure 2. NMR and MS spectra of compound **3**.









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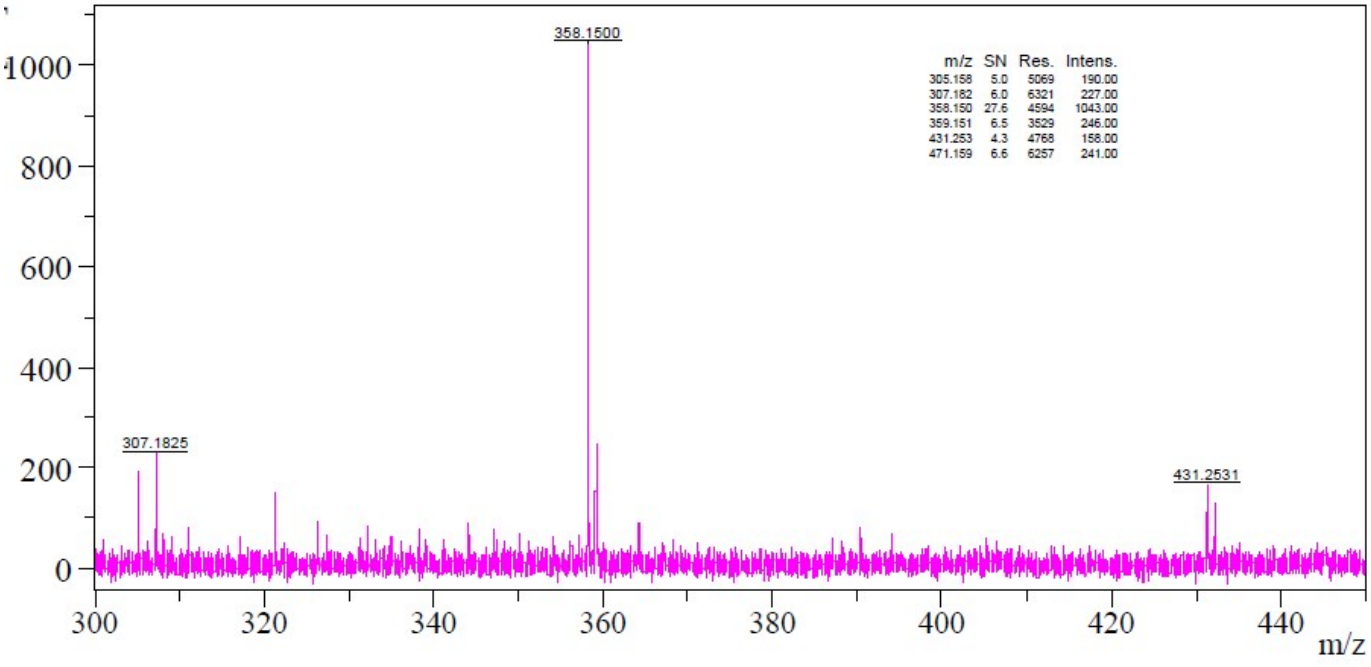


12-Cyclopenthyl-12,13,13b,13c-tetrahydro-6*H*,11*H*,14*H*-4b,5a,10b,12,13a-pentaazadibenzo[*a,h*]cyclohepta[*1,2,3,4-def*]fluorene (**4**).

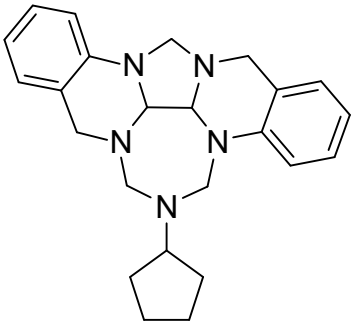
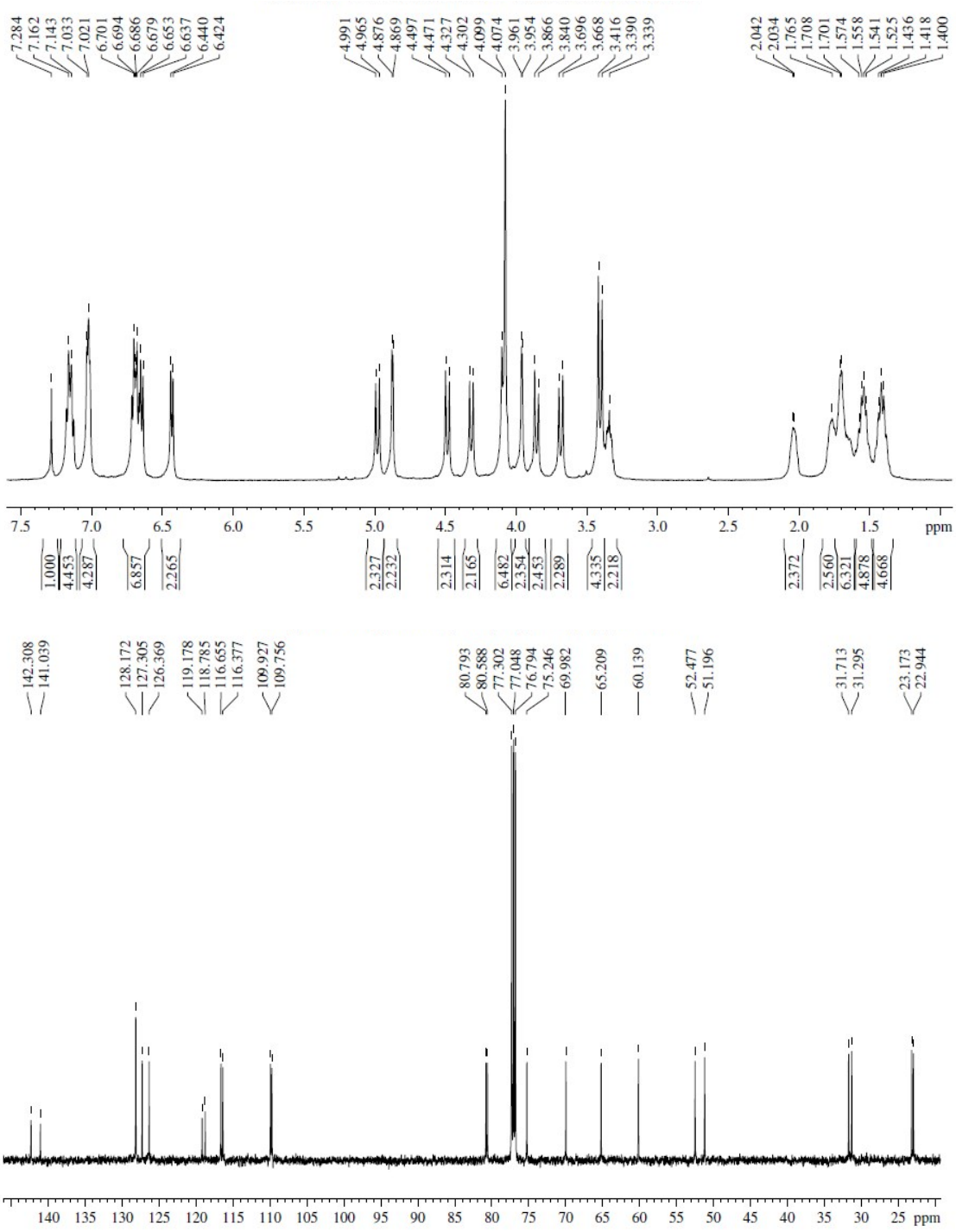
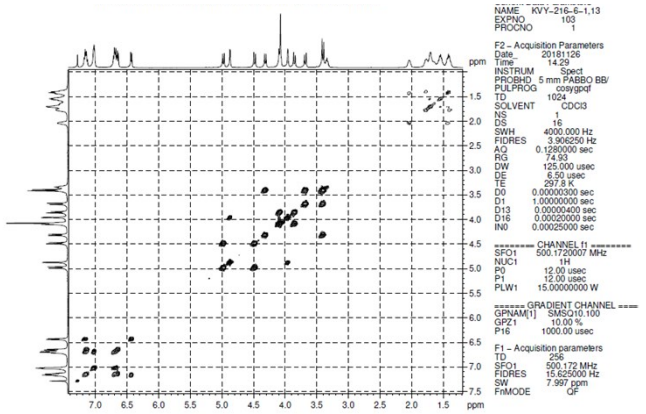
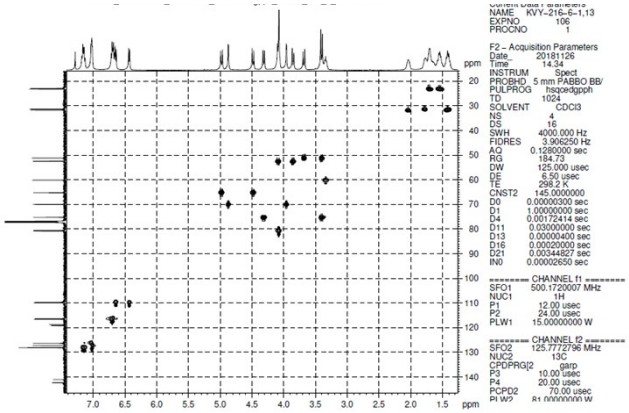
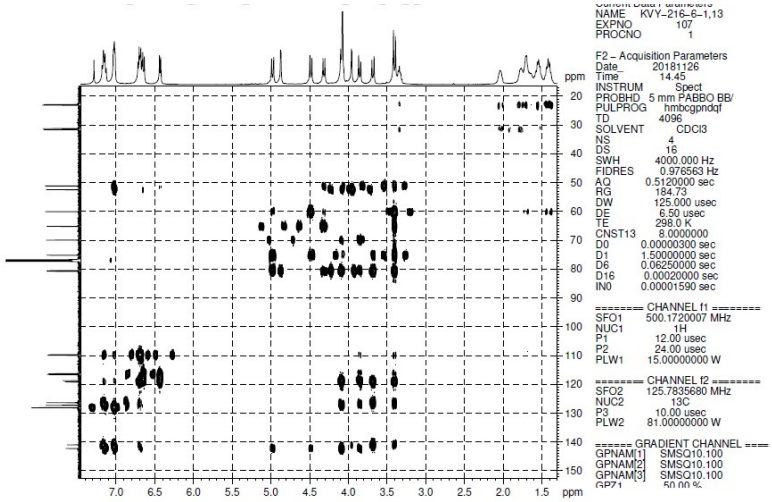


Figure 3. NMR and MS spectra of compound **4**.









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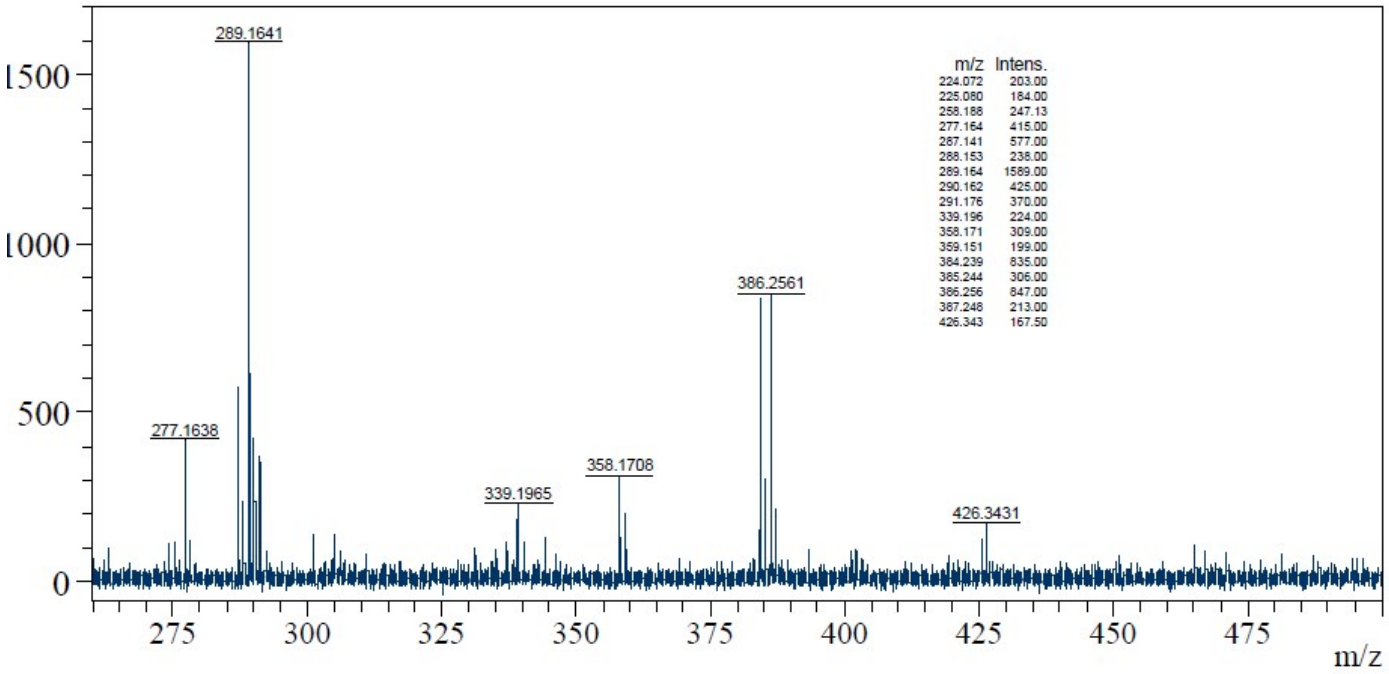
Comment 2 SA RP



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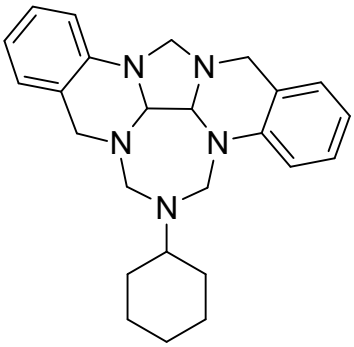

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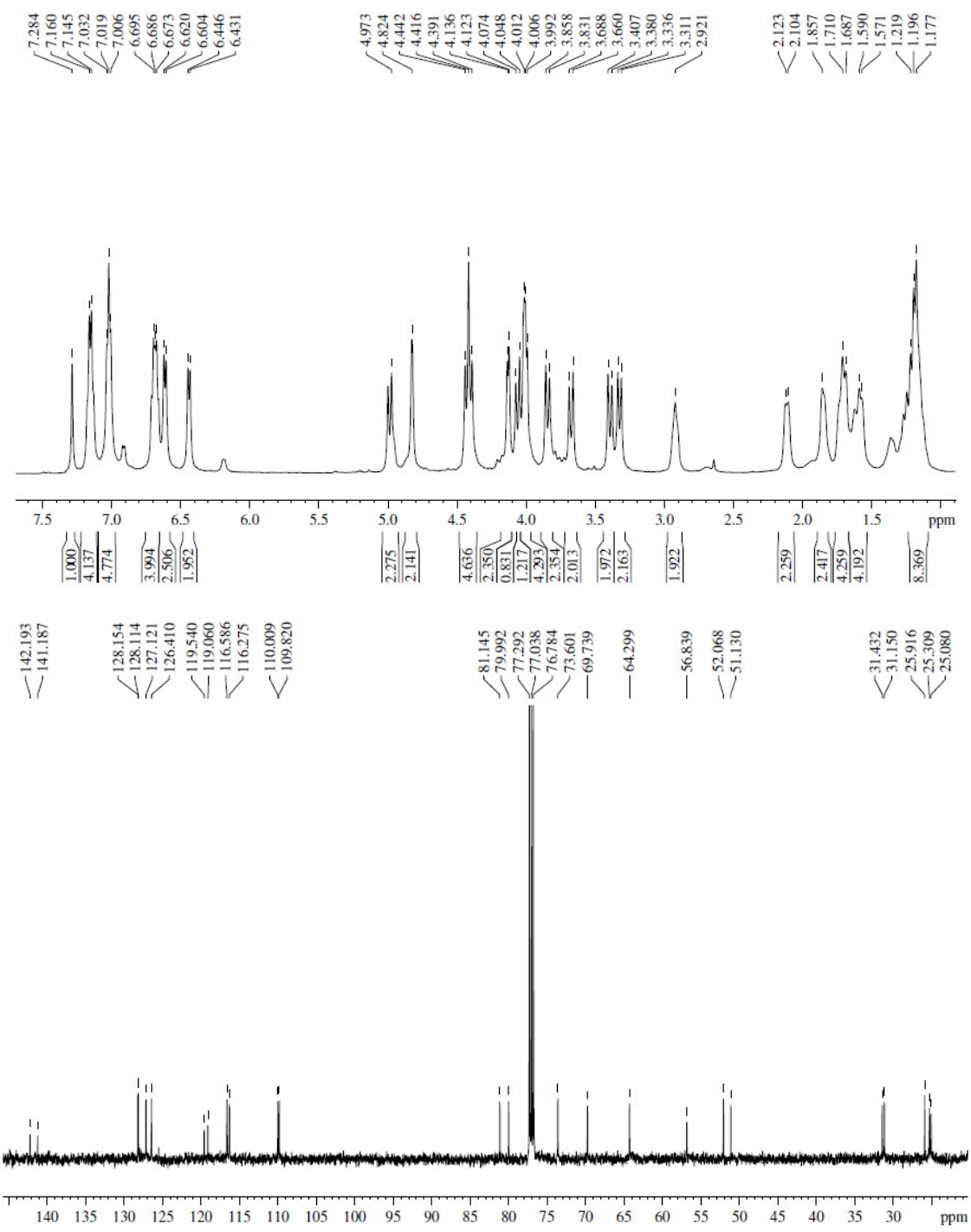

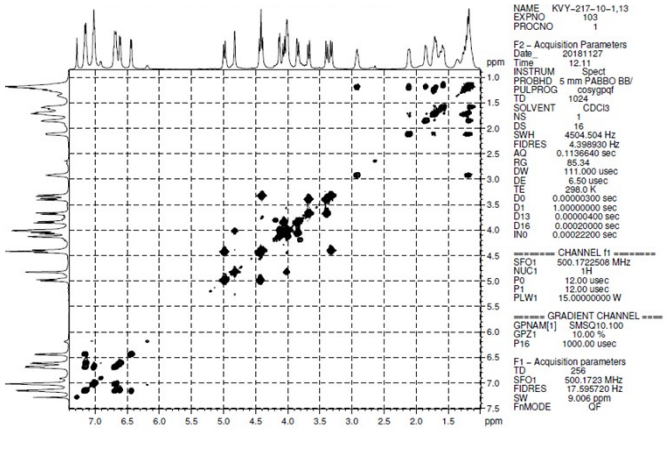

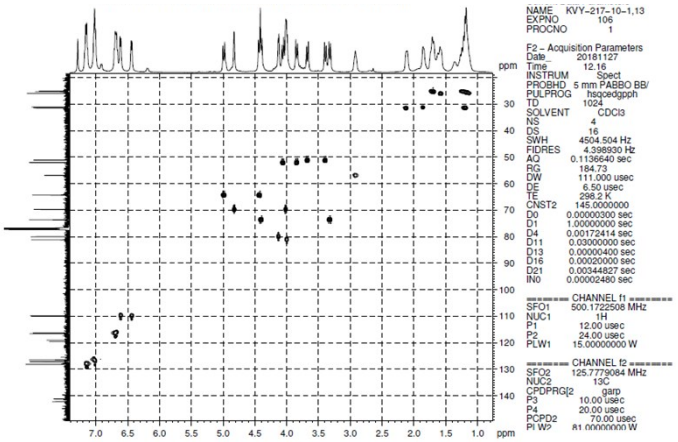

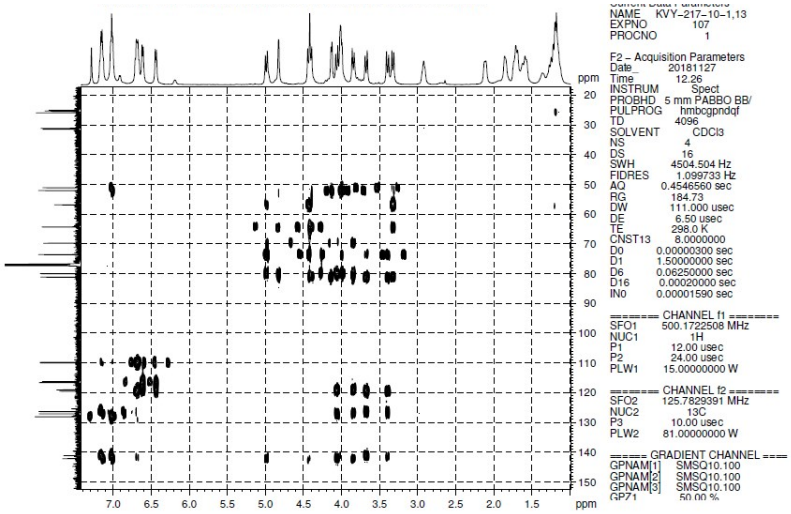

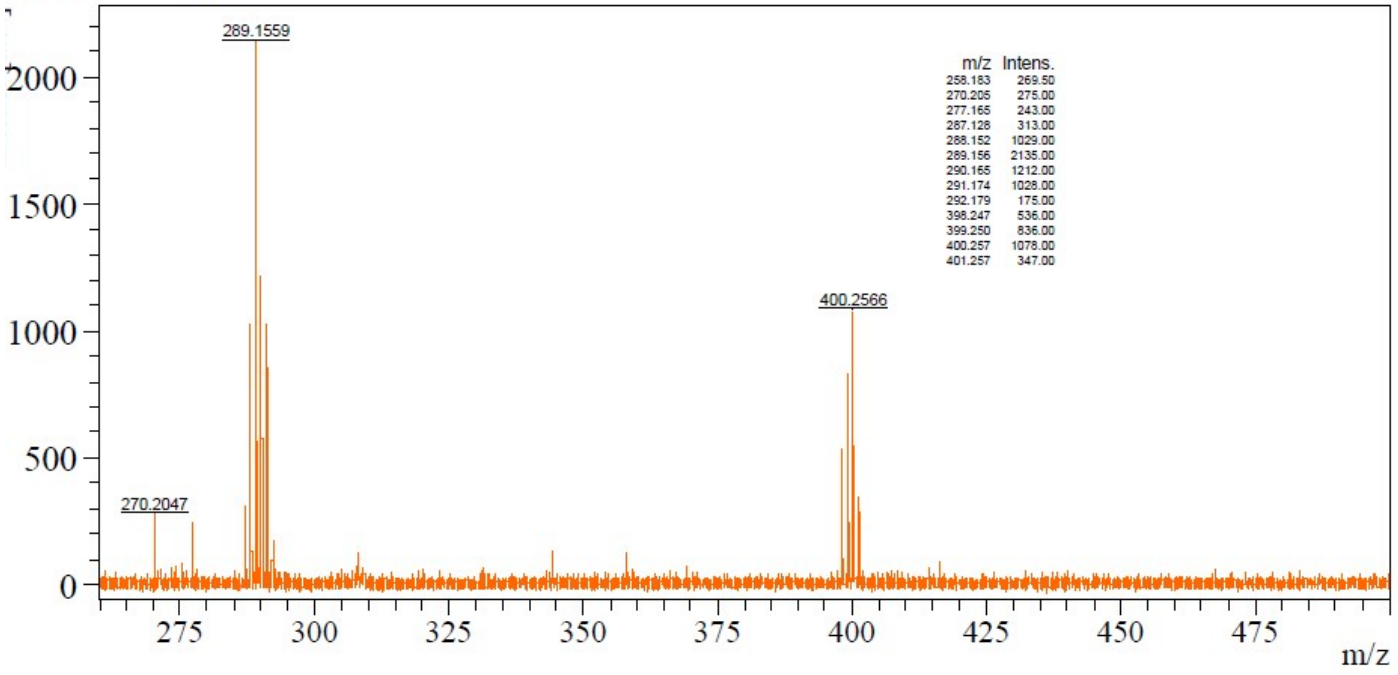
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292.179 175.00
398.247 536.00
399.250 836.00
400.257 1078.00
401.257 347.00
m/z

12-Cycloheptyl-12,13,13b,13c-tetrahydro-6*H*,11*H*,14*H*-4b,5a,10b,12,13a-pentaazadibenzo[*a,h*]cyclohepta[*1,2,3,4-def*]fluorene (**6**).

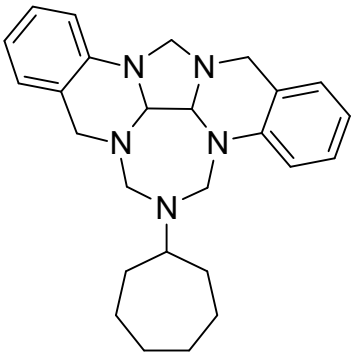
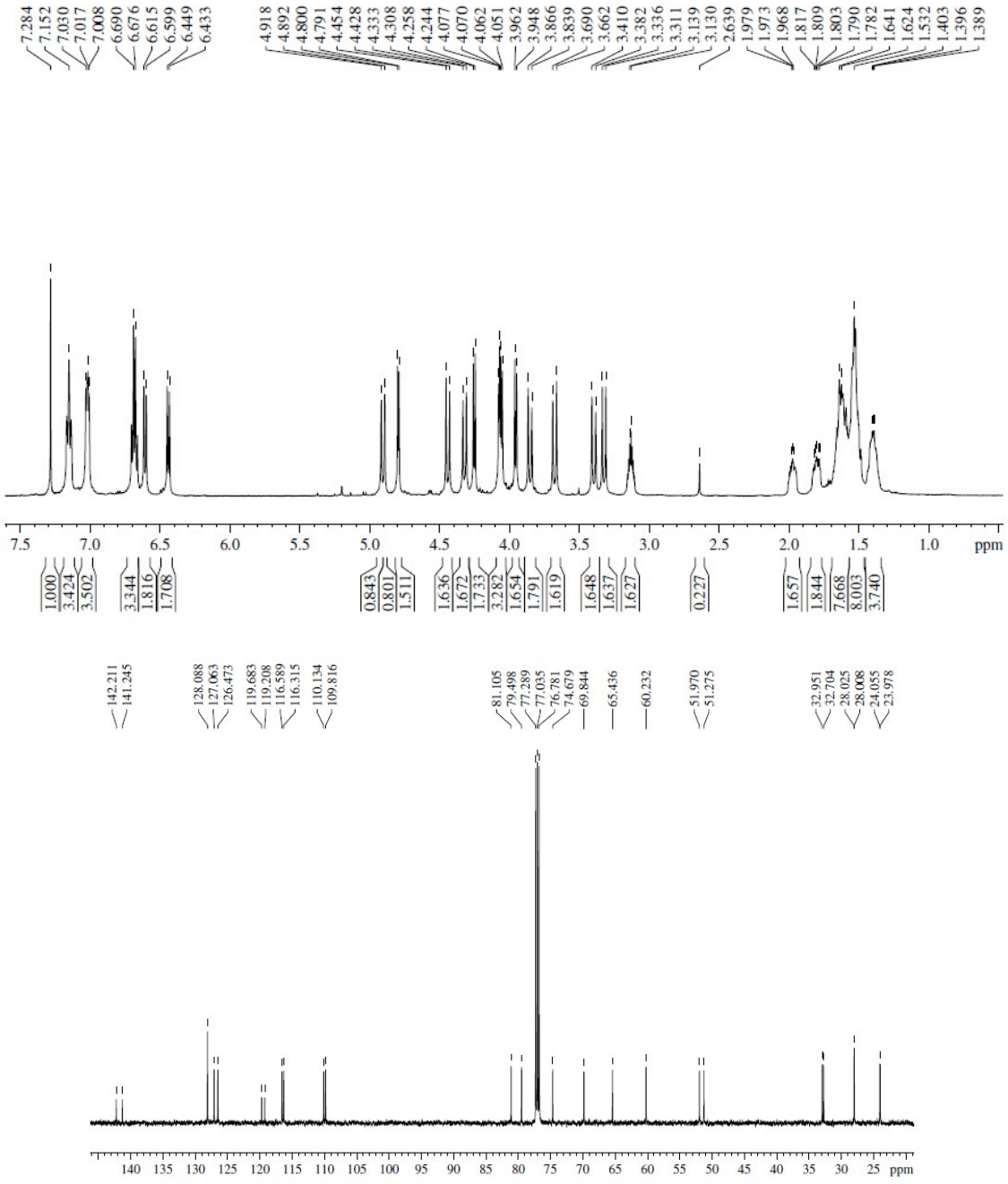
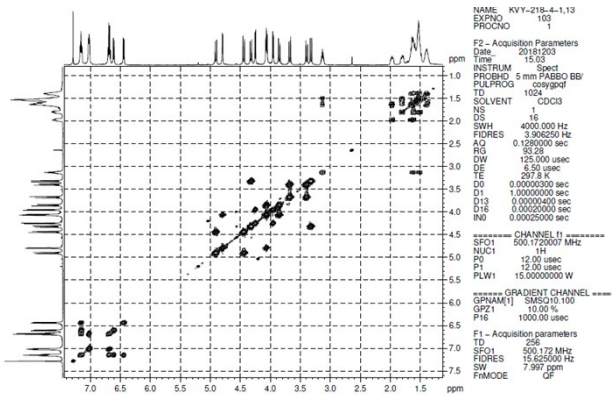


Figure 5. NMR spectra of compound **6**.





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TD 1024
SOLVENT CDCl3
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DS 16
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FIDRES 3.906250 Hz
AQ 0.1280000 sec
RG 93.28
DW 125.000 usec
DE 6.50 usec
TE 297.8 K
D0 0.00000300 sec
D1 1.00000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00025000 sec

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NUC1 1H
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P1 12.00 usec
PLW1 15.00000000 W

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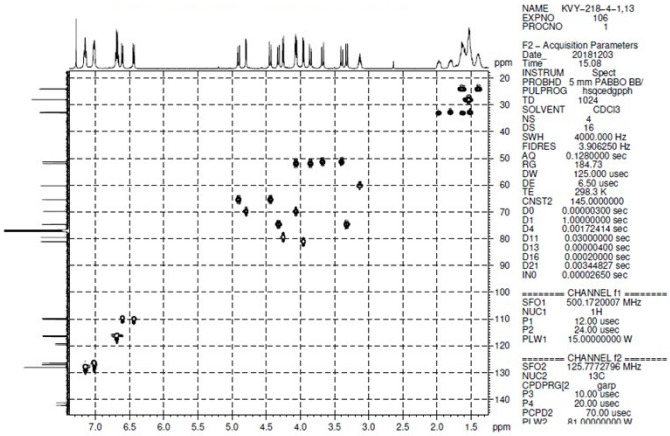
FIDRES 15.625000 Hz
SW 7.997 ppm
FnMODE QF



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SOLVENT CDCl3
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DS 16
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FIDRES 3.906250 Hz
AQ 0.1280000 sec
RG 184.73
DW 125.000 usec
DE 6.50 usec
TE 298.3 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.00000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
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D16 0.00020000 sec
D21 0.00344827 sec
IN0 0.00002650 sec

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NUC1 1H
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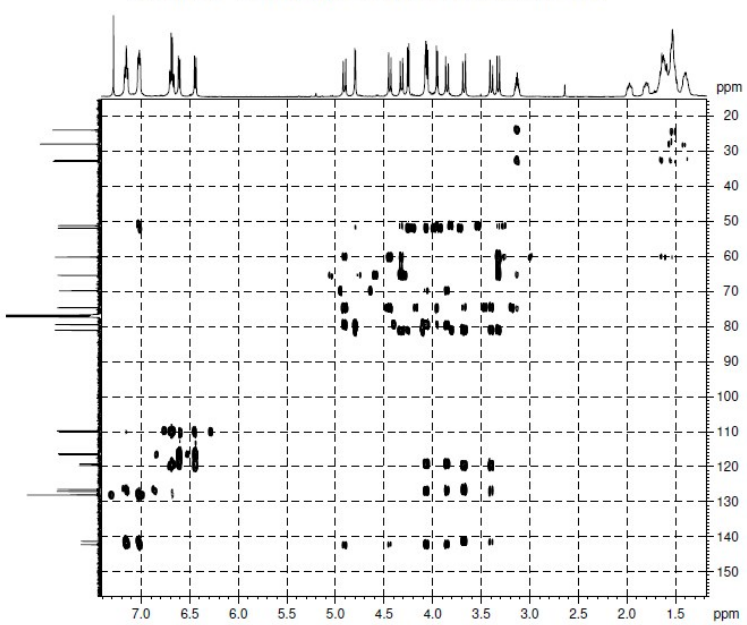

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SOLVENT CDCl3
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FIDRES 0.976563 Hz
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RG 184.73
DW 125.000 usec
DE 6.50 usec
TE 298.0 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00001590 sec

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NUC1 1H
P1 12.00 usec
P2 24.00 usec
PLW1 15.00000000 W

======== CHANNEL f2 ========
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NUC2 13C
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PLW2 81.00000000 W

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12-Cyclooctyl-12,13,13b,13c-tetrahydro-6*H*,11*H*,14*H*-4b,5a,10b,12,13a-pentaazadibenzo[*a,h*]cyclohepta[*1,2,3,4-def*]fluorene (**7**).

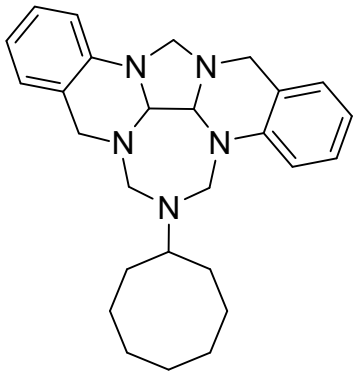
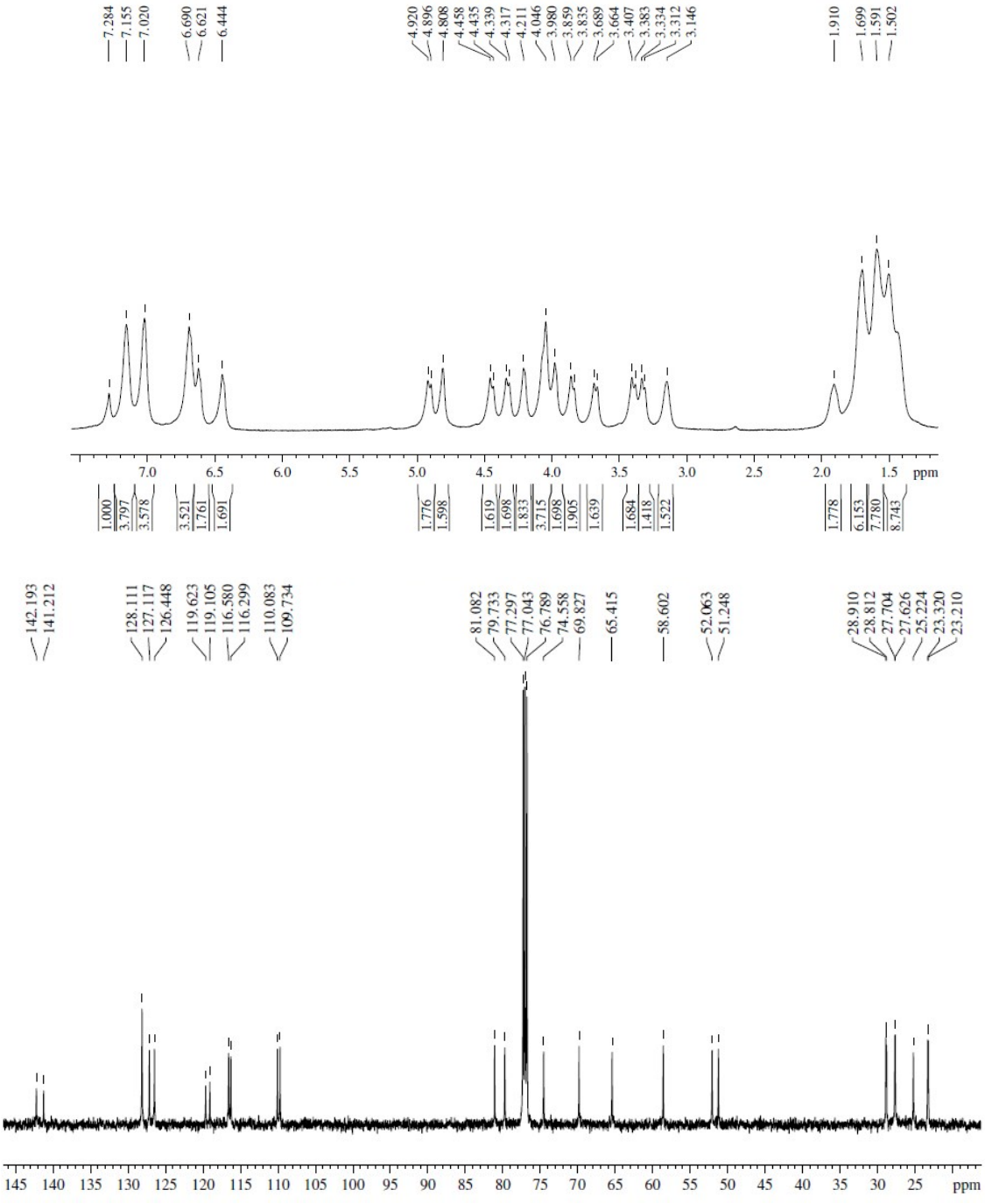
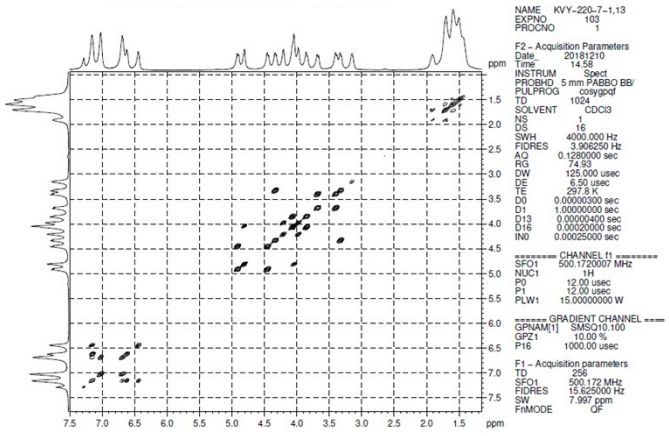
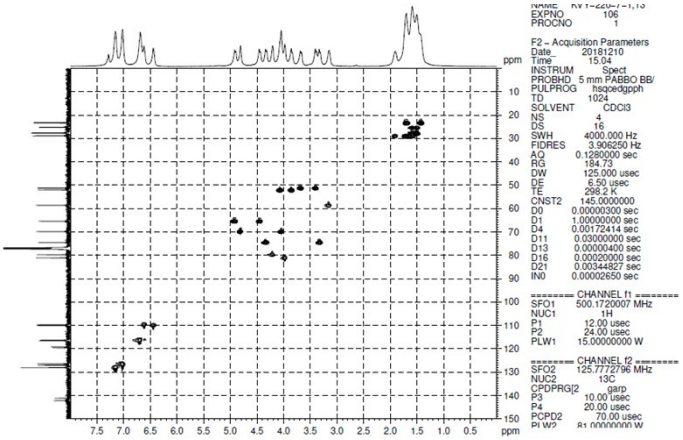
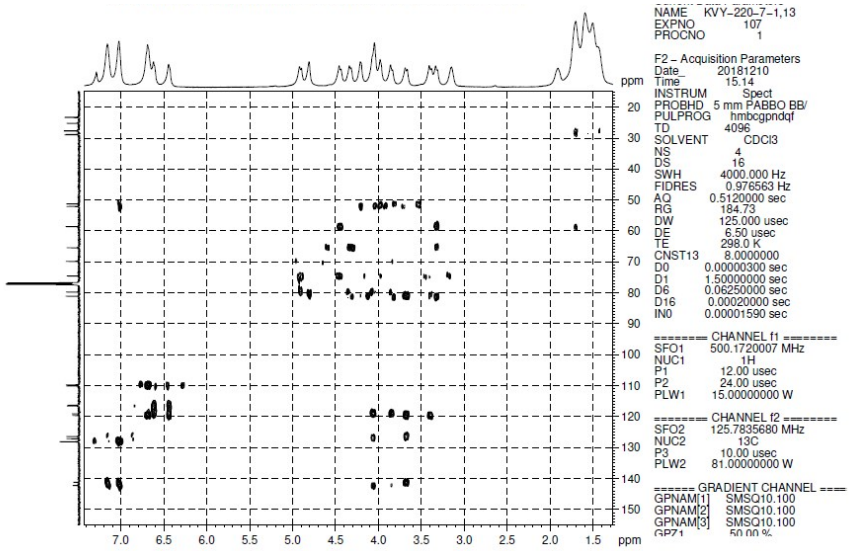


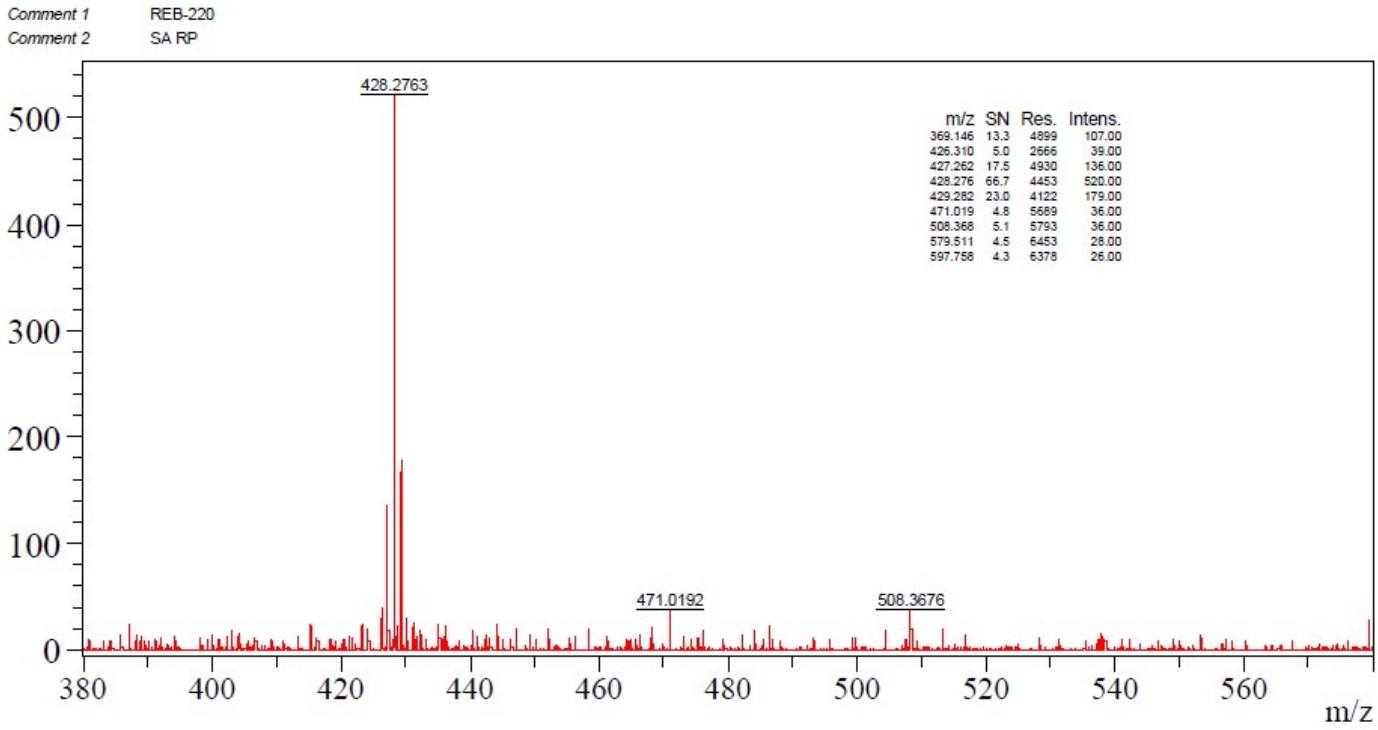
Figure 6. NMR and MS spectra of compound **7**.







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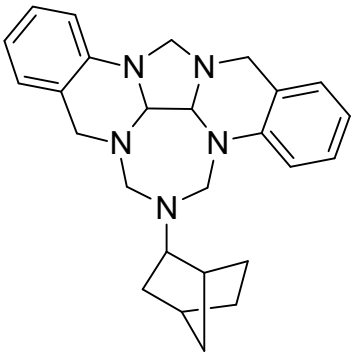
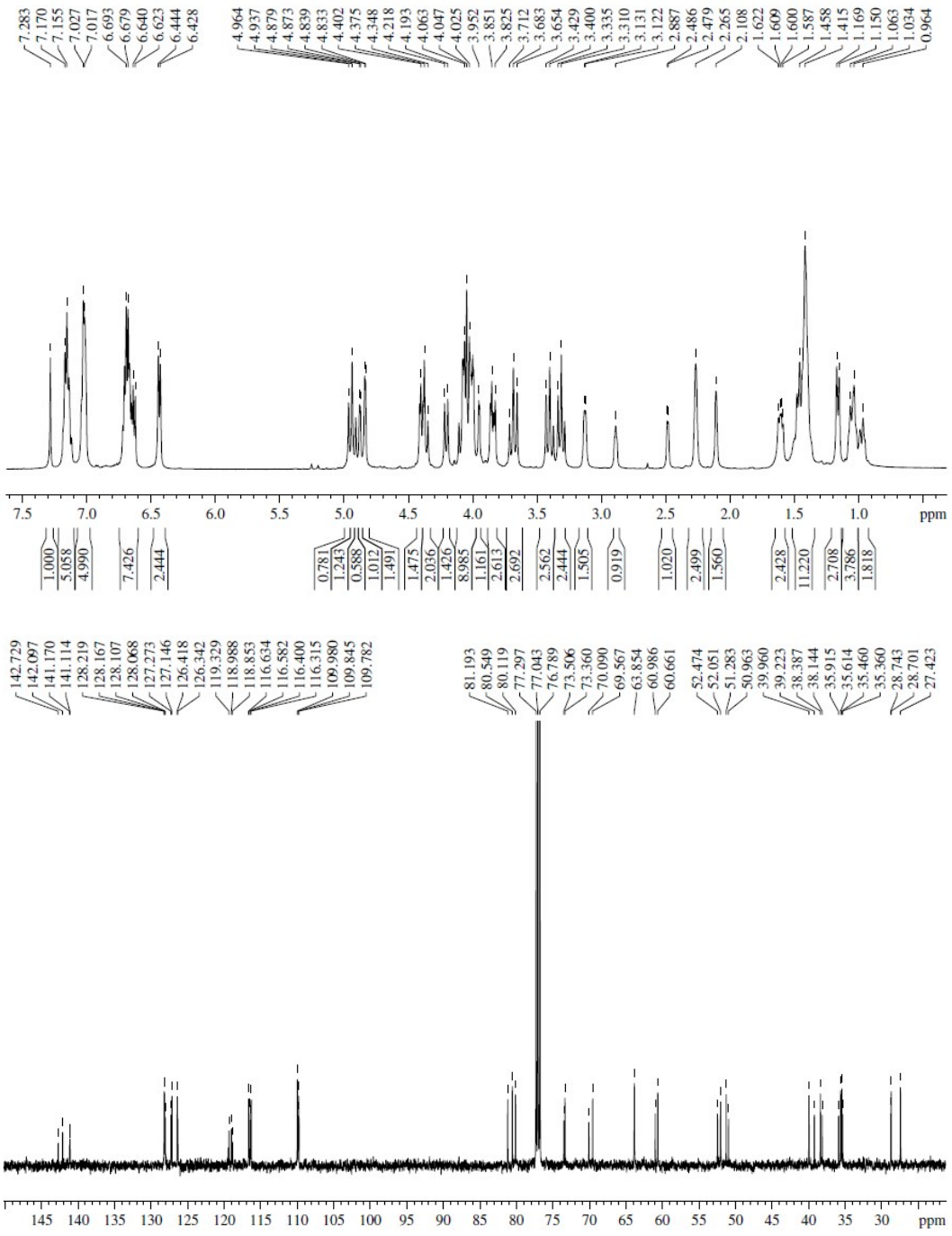
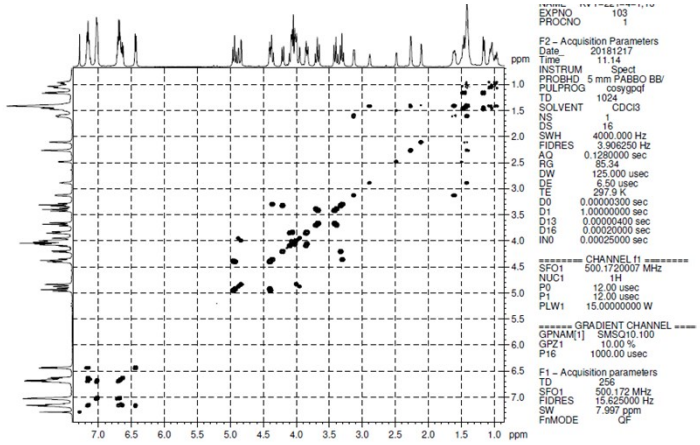


Figure 7. NMR and MS spectra of compound **8**.





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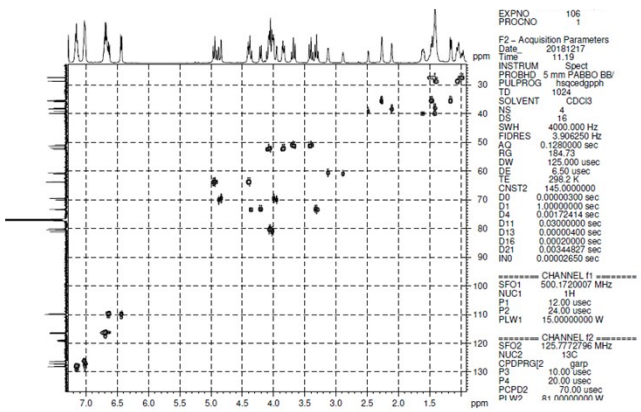

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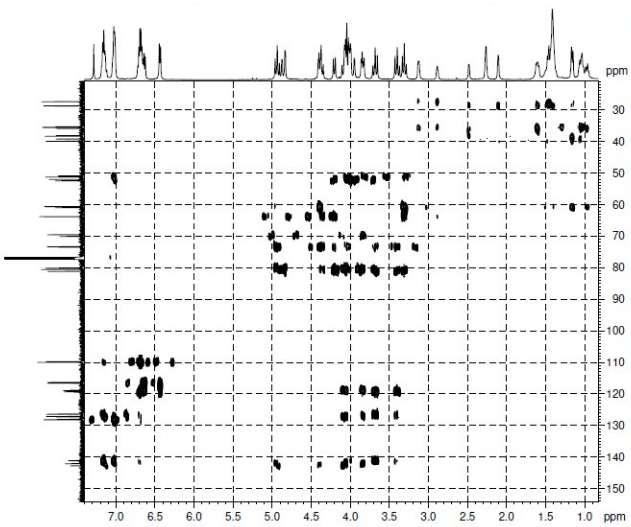

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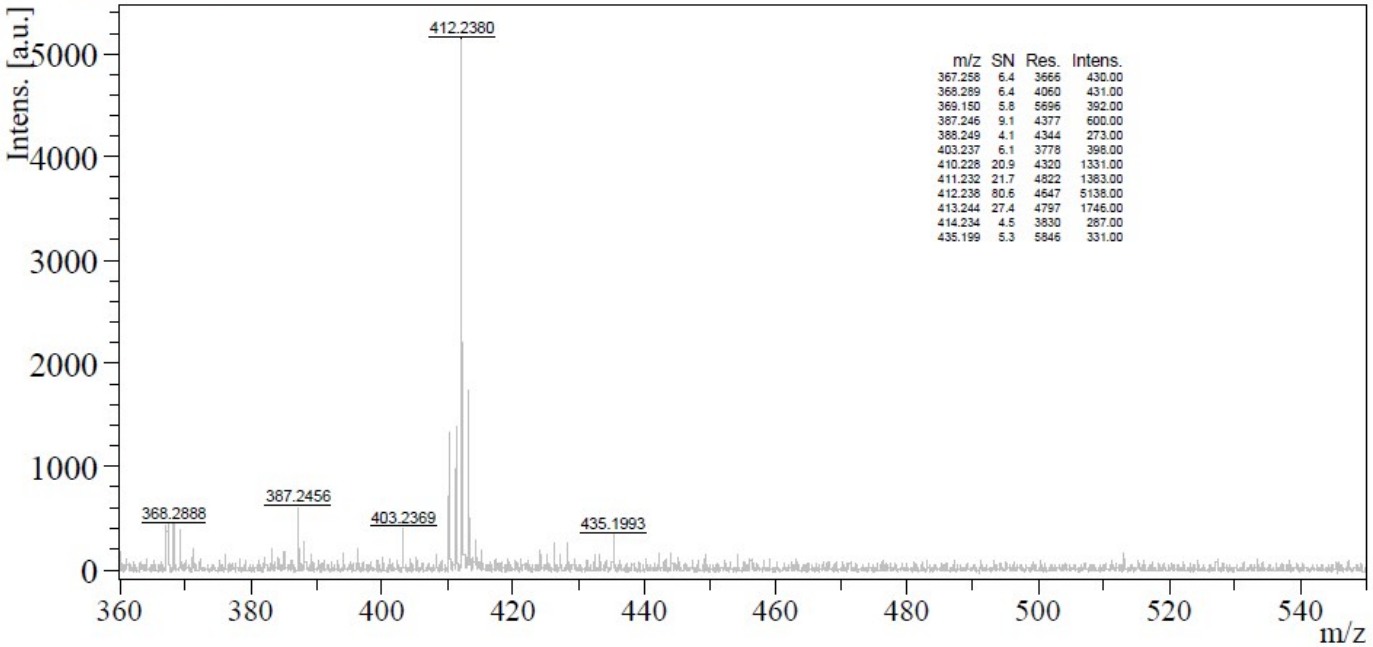
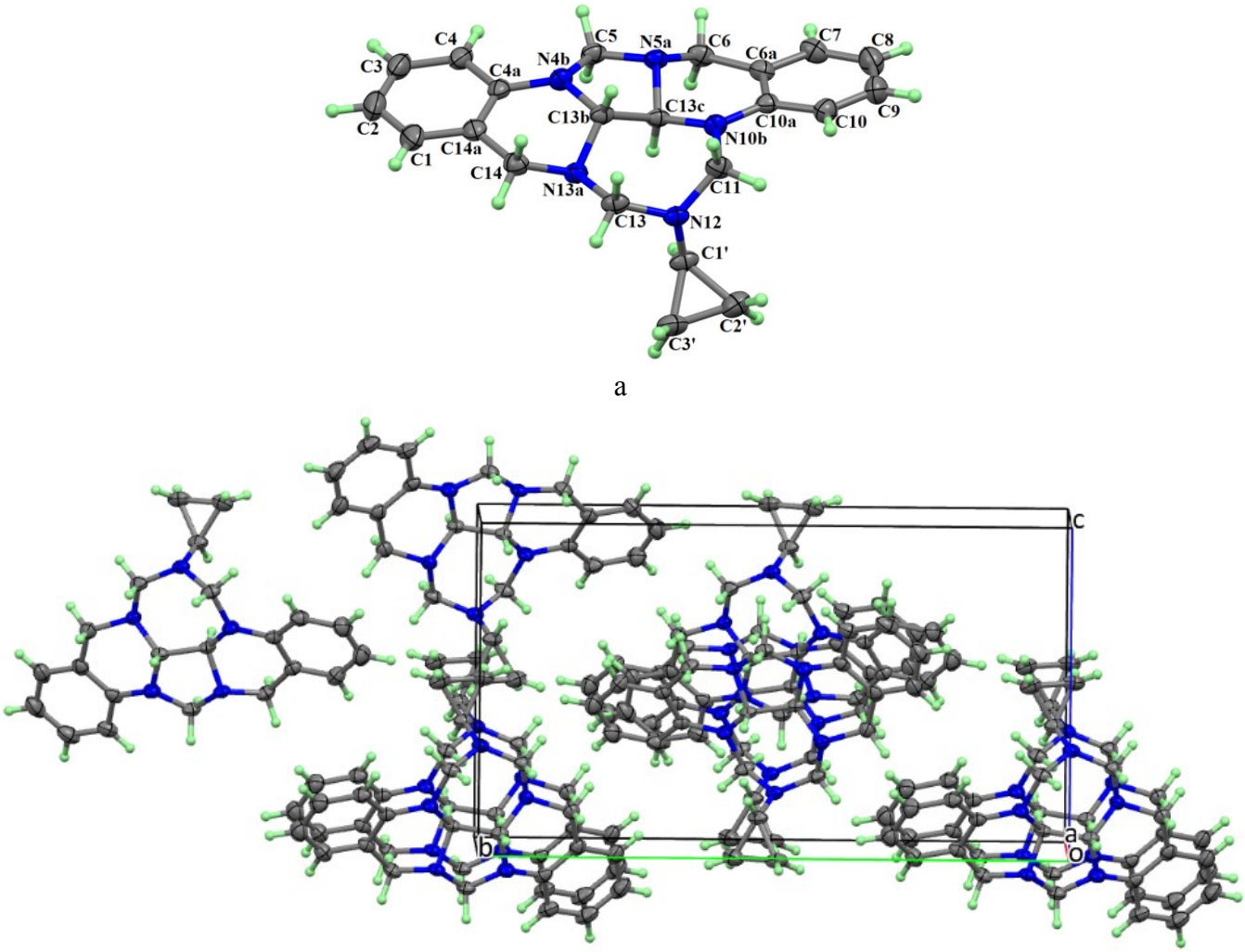
Comment 2 SA RP



m/z	SN	Res.	Intens.
367.258	6.4	3666	430.00
368.289	6.4	4060	431.00
369.150	5.8	5696	392.00
387.246	9.1	4377	600.00
388.249	4.1	4344	273.00
403.237	6.1	3778	398.00
410.228	20.9	4320	1331.00
411.232	21.7	4822	1383.00
412.238	80.6	4647	5138.00
413.244	27.4	4797	1746.00
414.234	4.5	3830	287.00
435.199	5.3	5846	331.00

X-ray data of compound **3**

Figure 8. (a) The asymmetric unit of compound **3**. Non-hydrogen atoms are represented by thermal ellipsoids (p = 30%) (b) The part of the crystal structure **3**, view along a axis.



a

b

Table 1. Crystal data and structure refinement for compound **3**.

CCDC	1990121
Empirical formula	$C_{22}H_{25}N_5$
Formula weight	359.47
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	9.5806(4)
b/Å	18.4584(9)
c/Å	10.4334(4)
α/°	90
β/°	91.070(4)

γ/°	90
Volume/Å^3	1844.74(14)
Z	4
ρ_{calc}g/cm^3	1.294
μ/mm^{-1}	0.079
F(000)	768.0
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.79 to 58.022
Indexranges	-7 ≤ h ≤ 12, -13 ≤ k ≤ 24, -14 ≤ l ≤ 14
Reflectionscollected	8627
Independentreflections	4221 [R_{int} = 0.0219]
Data/restraints/parameters	4221/0/244
Goodness-of-fit on F^2	1.019
Final R indexes [I>=2σ (I)]	R_1 = 0.0479, wR_2 = 0.1079
Final R indexes [all data]	R_1 = 0.0880, wR_2 = 0.1270
Largest diff. peak/hole / e Å^{-3}	0.14/-0.18

Table 2. Bond Lengths for compound **3**, Å.

Bond		Bond	
N5A–C13C	1.4542(17)	C13C–C13B	1.511(2)
N5A–C6	1.4487(19)	C6A–C6	1.495(2)
N5A–C5	1.4436(19)	C6A–C7	1.384(2)
C10A–N10B	1.386(2)	C4A–C14A	1.397(2)
C10A–C6A	1.404(2)	C4A–C4	1.396(2)
C10A–C10	1.398(2)	C14–C14A	1.490(2)
N12–C13	1.429(2)	C14A–C1	1.377(2)
N12–C11	1.4266(19)	C4–C3	1.373(2)
N12–C1'	1.4224(19)	C10–C9	1.378(2)
N13A–C13B	1.4526(18)	C1'–C3'	1.485(2)
N13A–C14	1.469(2)	C1'–C2'	1.493(2)
N13A–C13	1.4714(18)	C7–C8	1.377(2)
N10B–C13C	1.4419(18)	C1–C2	1.380(3)
N10B–C11	1.4663(18)	C3'–C2'	1.480(3)
N4B–C13B	1.4601(18)	C9–C8	1.364(3)
N4B–C4A	1.3733(19)	C3–C2	1.373(3)
N4B–C5	1.443(2)		

Table 3. Bond Angles for compound **3**,°

Angle		Angle	
C6–N5A–C13C	111.64(11)	N4B–C13B–C13C	100.98(11)
C5–N5A–C13C	103.73(11)	N5A–C6–C6A	108.98(12)

C5–N5A–C6	115.02(12)	N4B–C4A–C14A	118.86(15)
N10B–C10A–C6A	119.96(14)	N4B–C4A–C4	121.49(16)
N10B–C10A–C10	122.12(14)	C4–C4A–C14A	119.63(16)
C10–C10A–C6A	117.88(16)	N13A–C14–C14A	111.04(13)
C11–N12–C13	117.66(13)	C4A–C14A–C14	118.87(15)
C1'–N12–C13	117.45(13)	C1–C14A–C4A	118.73(17)
C1'–N12–C11	116.80(14)	C1–C14A–C14	122.40(17)
C13B–N13A–C14	109.25(12)	N12–C13–N13A	116.27(12)
C13B–N13A–C13	109.26(11)	N12–C11–N10B	115.95(12)
C14–N13A–C13	107.67(12)	C3–C4–C4A	120.24(19)
C10A–N10B–C13C	118.28(12)	C9–C10–C10A	120.71(17)
C10A–N10B–C11	122.16(12)	N4B–C5–N5A	101.93(11)
C13C–N10B–C11	117.94(12)	N12–C1'–C3'	117.72(14)
C4A–N4B–C13B	121.96(13)	N12–C1'–C2'	117.13(14)
C4A–N4B–C5	123.03(13)	C3'–C1'–C2'	59.60(11)
C5–N4B–C13B	110.68(12)	C8–C7–C6A	121.82(17)
N5A–C13C–C13B	101.26(11)	C14A–C1–C2	121.4(2)
N10B–C13C–N5A	109.36(11)	C2'–C3'–C1'	60.48(11)
N10B–C13C–C13B	116.90(12)	C8–C9–C10	121.28(18)
C10A–C6A–C6	120.55(15)	C3'–C2'–C1'	59.92(11)
C7–C6A–C10A	119.44(15)	C9–C8–C7	118.68(19)
C7–C6A–C6	119.97(14)	C2–C3–C4	120.22(19)
N13A–C13B–N4B	111.40(12)	C3–C2–C1	119.75(19)
N13A–C13B–C13C	114.19(12)		

Table 4. Interaction Energies [E_{int}] for the Main Hyperconjugative Interactions in compound **3**.

Interaction	E_{int}, kcal/mol	Interaction	E_{int}, kcal/mol
$LP(N^{12}) \rightarrow \sigma^*(C^{11}–N^{10b})$	15.60	$LP(N^{12}) \rightarrow \sigma^*(C^{13}–N^{13a})$	14.49
$LP(N^{10b}) \rightarrow \sigma^*(C^{11}–N^{12})$	3.76	$LP(N^{13a}) \rightarrow \sigma^*(C^{13}–N^{12})$	1.18
$LP(N^{10b}) \rightarrow \sigma^*(C^{10a}–C^{10})$	41.62	$LP(N^{4b}) \rightarrow \sigma^*(C^{4a}–C^{14a})$	38.47
$LP(N^{10b}) \rightarrow \sigma^*(N^{5a}–C^{13c})$	2.94	$LP(N^{4b}) \rightarrow \sigma^*(N^{13a}–C^{13b})$	4.52
$LP(N^{13a}) \rightarrow \sigma^*(N^{4b}–C^{13b})$	1.02	$LP(N^{5a}) \rightarrow \sigma^*(C^{13c}–N^{10b})$	2.49
$LP(N^{5a}) \rightarrow \sigma^*(C^{13c}–H^{13c})$	6.06	$LP(N^{5a}) \rightarrow \sigma^*(C^{5}–H^{5b})$	5.96
$LP(N^{5a}) \rightarrow \sigma^*(C^{5}–H^{5a})$	2.15		

Table 5. The Some of Geometric parameters (Å, °) for compound **3**.

$N^{4b}–C^{4a}$	1.373 Å	$N^{13a}–C^{14}$	1.469 Å	$N^{5a}–C^{5}$	1.444 Å	$N^{10b}–C^{13c}$	1.442 Å
$N^{4b}–C^{5}$	1.444 Å	$N^{13a}–C^{13}$	1.471 Å	$N^{5a}–C^{6}$	1.449 Å	$N^{10b}–C^{11}$	1.466 Å
$N^{4b}–C^{13b}$	1.460 Å	$N^{12}–C^{13}$	1.429 Å	$N^{5a}–C^{13c}$	1.454 Å	$N^{12}–C^{11}$	1.427 Å
$N^{13a}–C^{13b}$	1.453 Å	$N^{12}–C^{1'}$	1.422 Å	$N^{10b}–C^{10a}$	1.386 Å	$\sum_{\angle N12}$	351.9°
$\sum_{\angle N4b}$	355.65°	$\sum_{\angle N5a}$	330.39°	$\sum_{\angle N13a}$	326.19°	$\sum_{\angle N10b}$	358.38°

Table 6. Topological parameters of electron density at the (3, –1) BCPs of compound **3**.

Bond	$\rho(r)$, e/au^3	$-\nabla^2\rho(r)$, e/au^5	ε	Bond	$\rho(r)$, e/au^3	$-\nabla^2\rho(r)$, e/au^5	ε
C^1–C^2	0.3180	0.8377	0.5006	C^{11}–N^{12}	0.2906	0.9783	0.0254
C^2–C^3	0.3230	1.0861	0.0382	N^{12}–C^{13}	0.2884	0.9616	0.0135
C^3–C^4	0.3220	0.8619	0.3018	C^{13}–N^{13a}	0.2717	0.8315	0.0571
C^4–C^{4a}	0.3109	0.9916	0.0531	N^{13a}–C^{14}	0.2715	0.8148	0.0207
C^{4a}–N^{4b}	0.3126	1.1312	0.0189	C^{14}–C^{14a}	0.2672	0.6907	0.0239
N^{4b}–C^5	0.2794	0.8903	0.0426	C^{14a}–C^1	0.3211	1.0485	0.0421
C^5–N^{5a}	0.2896	0.9342	0.0449	N^{10b}–C^{13c}	0.2814	0.8719	0.0378
N^{5a}–C^6	0.2784	0.8861	0.0175	C^{13b}–C^{13c}	0.2664	0.6944	0.0072
C^6–C^{6a}	0.2660	0.6865	0.0243	N^{13a}–C^{13b}	0.2853	0.8719	0.0494
C^{6a}–C^7	0.3166	0.8053	0.5120	N^{5a}–C^{13c}	0.2878	0.8762	0.0476
C^7–C^8	0.3207	1.0683	0.0376	N^{4b}–C^{13b}	0.2751	0.8053	0.0424
C^8–C^9	0.3283	0.9029	0.5121	C^{4a}–C^{14a}	0.3151	0.7847	0.5546
C^9–C^{10}	0.3190	1.0495	0.0430	N^{12}–$C^{1'}$	0.2897	0.9626	0.0342
C^{10}–C^{10a}	0.3094	0.7781	0.5300	$C^{1'}$–$C^{2'}$	0.2635	0.5565	0.1649
C^{6a}–C^{10a}	0.3092	0.9603	0.0555	$C^{2'}$–$C^{3'}$	0.2652	0.6727	0.1373
C^{10a}–N^{10b}	0.3062	1.1191	0.0170	$C^{3'}$–$C^{1'}$	0.2676	0.5828	0.1561
N^{10b}–C^{11}	0.2624	0.7927	0.0639				

Table 7. Topological parameters of electron density at the (3, –1) bond critical points for intermolecular interactions in crystal of **3**.

Bond	$\rho(r)$, e/au^3	$\nabla^2\rho(r)$, e/au^5	ε	E, kcal/mol
C^{11}–H^{11b}…N^{4b}	0.0071	0.0242	0.3612	1.47
C^{13b}–H^{13b}…$N1^{0b}$	0.0093	0.0296	0.0540	2.03
C^{13b}–H^{13b}…N^{5a}	0.0058	0.0214	1.6402	1.28
C^{13b}–H^{13b}…H^{13b}	0.0047	0.0188	1.5436	0.75
C^{13}–H^{13a}…N^{5a}	0.0035	0.0134	0.1917	0.63
C^{13c}–H^{13c}…π	0.0057	0.0155	0.2116	0.75
C^6–H^{6b}…π	0.0073	0.0241	2.1849	1.22
C^5–H^{5b}…π	0.0027	0.0080	0.9858	0.34
H^{5b}…H^{5b}	0.0030	0.0094	0.1218	0.41
H^{6a}…H^9	0.0078	0.0276	0.0661	1.50
H^7…H^{10}	0.0019	0.0058	0.0937	0.25