ELECTRONIC SUPPLEMENTARY MATERIALS

Synthesis, Structure, and Antitumor Activity of 2,9-Disubstituted Perhydro 2,3a,7b,9,10a,14b-Hexaazadibenzotetracenes

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Table of contents

(3b*R**,7a*R**,10b*R**,14a*R**)-2,9-Dipropyl-octadecahydro-1*H*,8*H*-2,3a,7b,9,10a,14b-hexaazadibenzo[*fg*,*op*]tetracene (**2**)

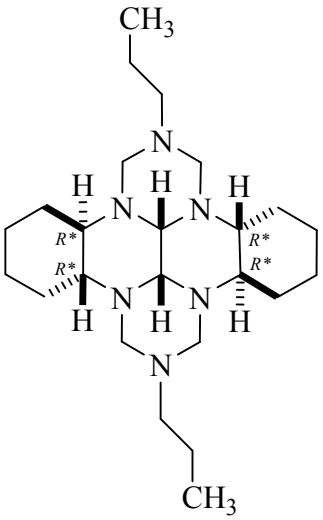
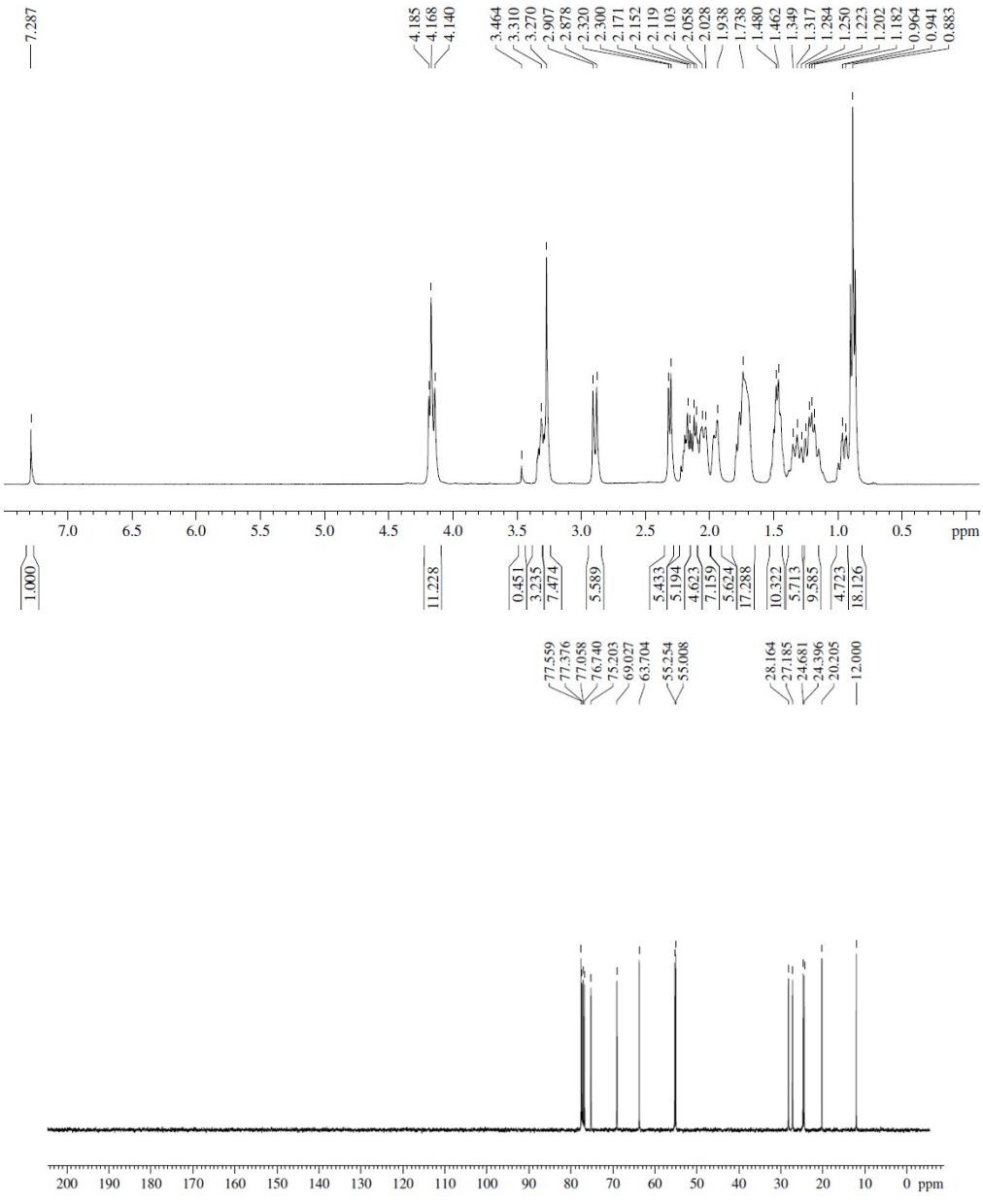
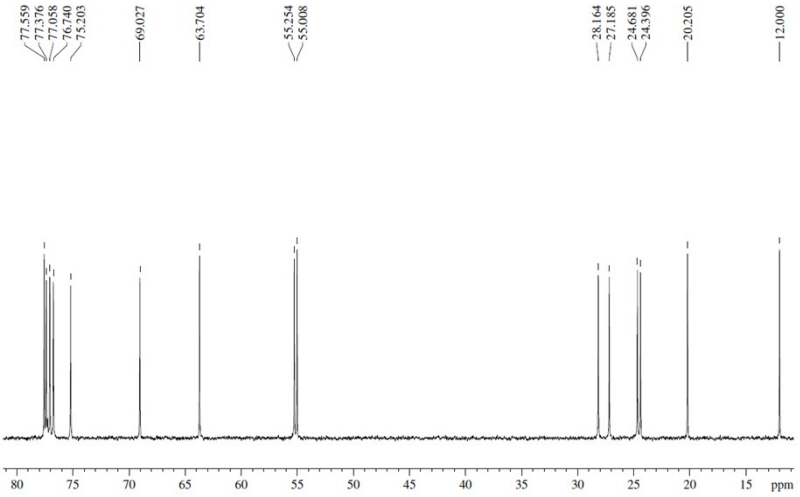


Figure 1. NMR and MS spectra of compound **2**.

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77.376
77.058
76.740
75.203
69.027
63.704
55.254
55.008
28.164
27.185
24.681
24.396
20.205
12.000
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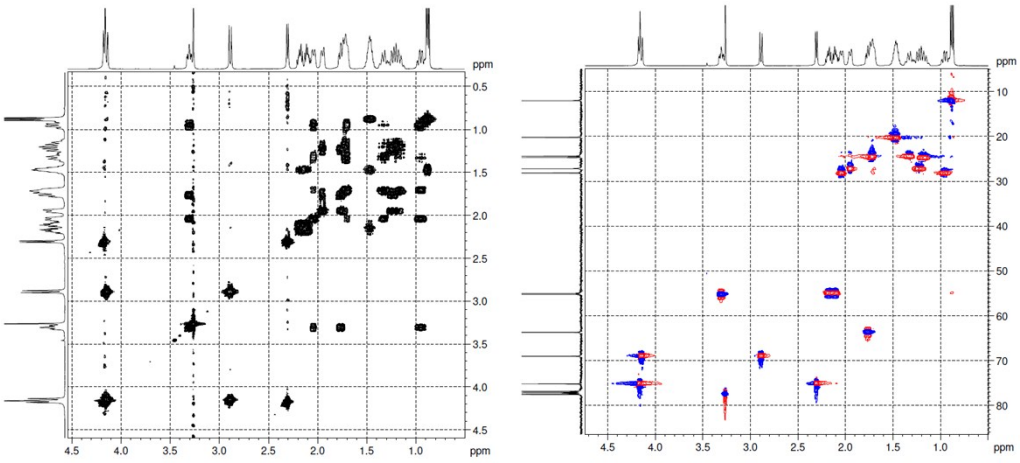
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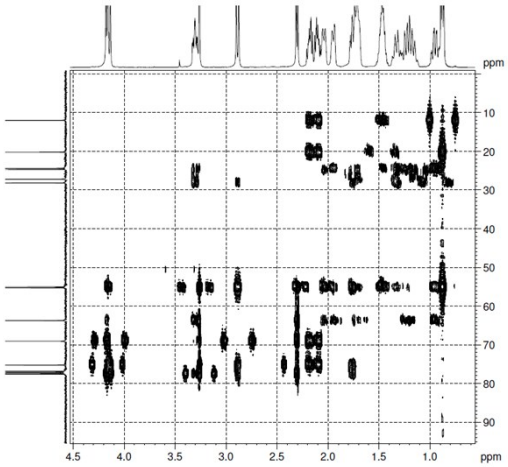
ppm
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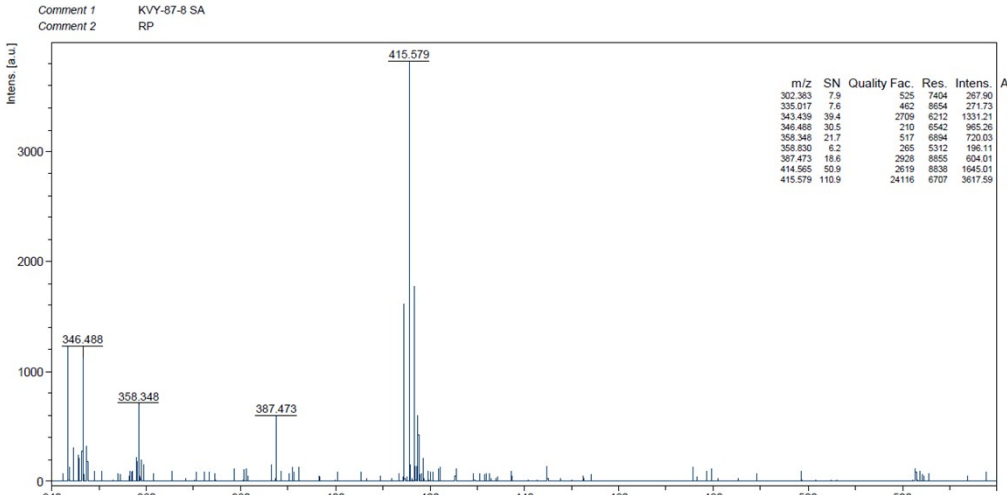
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Comment 2 RP
Intens. [a.u.]
415.579
346.488
358.348
387.473
m/z SN Quality Fac. Res. Intens. Area
302.383 7.9 525 7404 267.90 15
335.017 7.6 462 8654 271.73 15
343.439 39.4 2709 6212 1331.21 108
346.488 30.5 210 6542 965.26 69
358.348 21.7 517 6894 720.03 55
358.830 6.2 265 5312 196.11 18
387.473 18.6 2928 8855 604.01 39
414.565 50.9 2619 8838 1645.01 119
415.579 110.9 24116 6707 3617.59 329
340 360 380 400 420 440 460 480 500 520 m/z

(3b*R**,7a*R**,10b*R**,14a*R**)-2,9-Diisopropyl-octadecahydro-1*H*,8*H*-2,3a,7b,9,10a,14b-hexaazadibenzo[*fg*,*op*]tetracene (**3**)

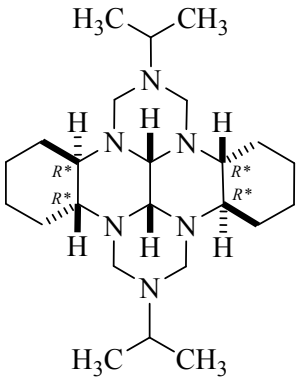
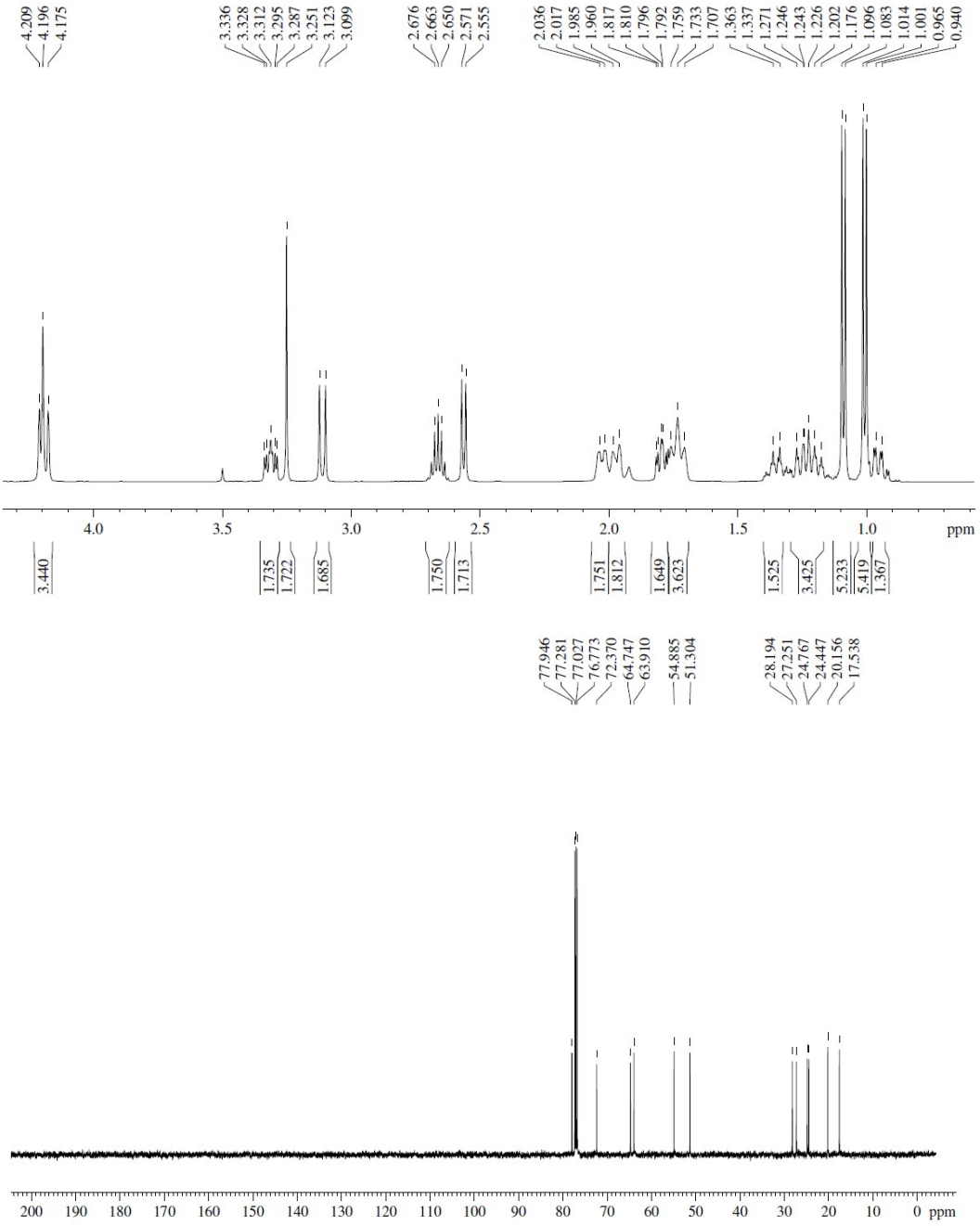
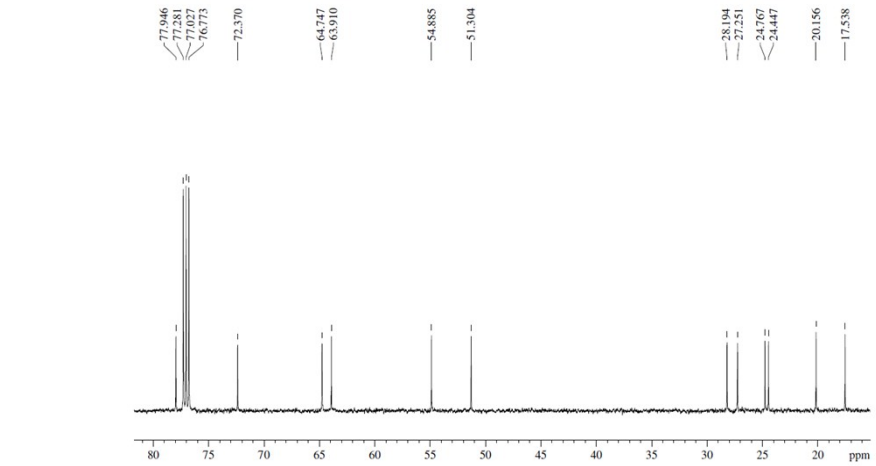
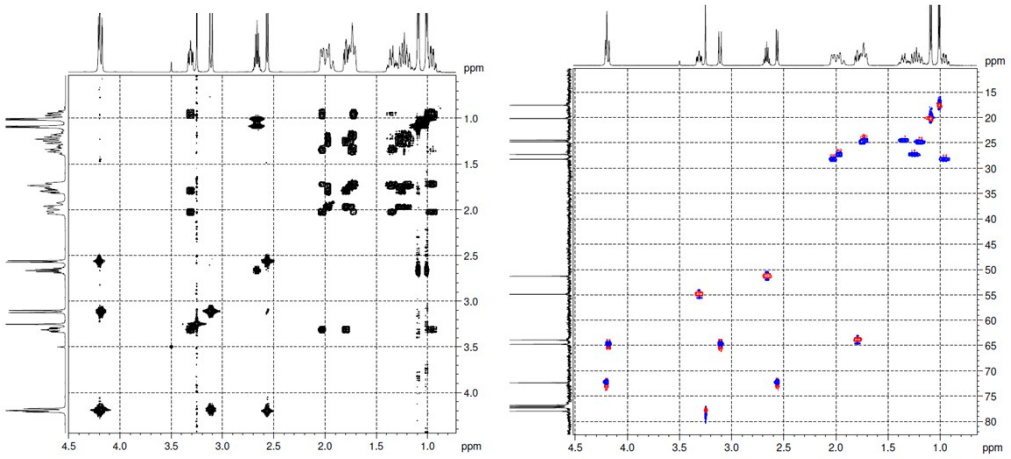
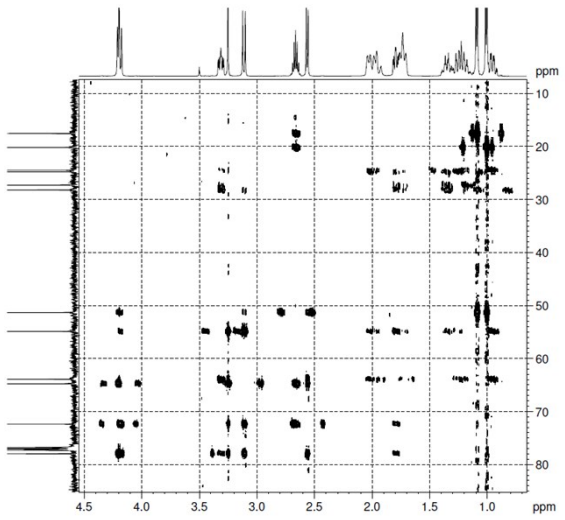


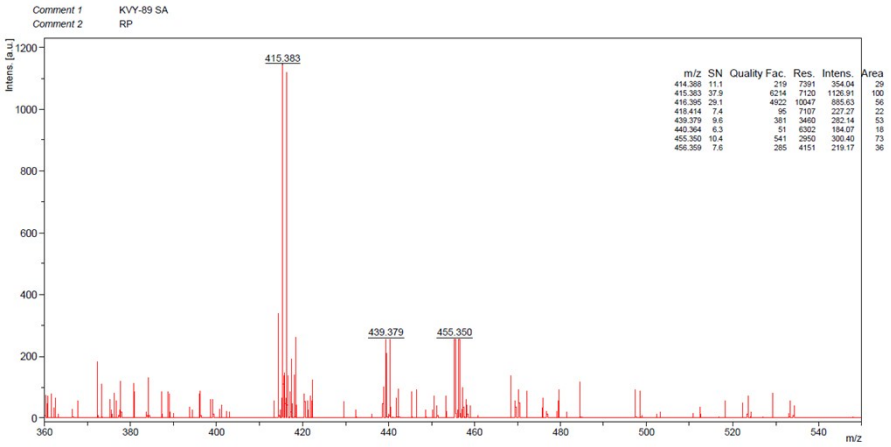
Figure 2. NMR and MS spectra of compound **3**.




77.946
77.281
77.027
76.773
72.370
64.747
63.910
54.885
51.304
28.194
27.251
24.767
24.447
20.156
17.538
80 75 70 65 60 55 50 45 40 35 30 25 20 ppm


ppm
4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
ppm
4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm


ppm
4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm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Comment 2 RP
Intens. [a.u.]
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439.379
455.350
m/z SN Quality Fac. Res. Intens. Area
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415.383 37.9 6214 7120 1126.91 100
416.395 29.1 4922 10047 885.63 56
418.414 7.4 95 7107 227.27 22
439.379 9.6 381 3460 282.14 53
440.364 6.3 51 6302 194.07 18
455.350 10.4 541 2950 300.40 73
456.359 7.6 285 4151 219.17 36
360 380 400 420 440 460 480 500 520 540 m/z

(3b*R**,7a*R**,10b*R**,14a*R**)-2,9-Dibutyl-octadecahydro-1*H*,8*H*-2,3a,7b,9,10a,14b-hexaazadibenzo[*fg*,*op*]tetracene (**4**)

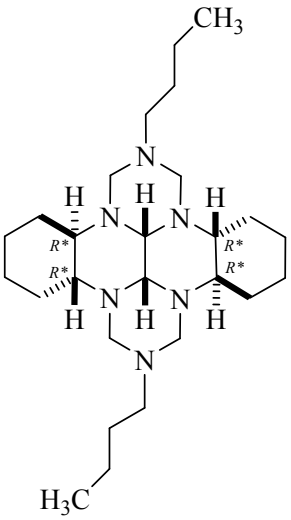
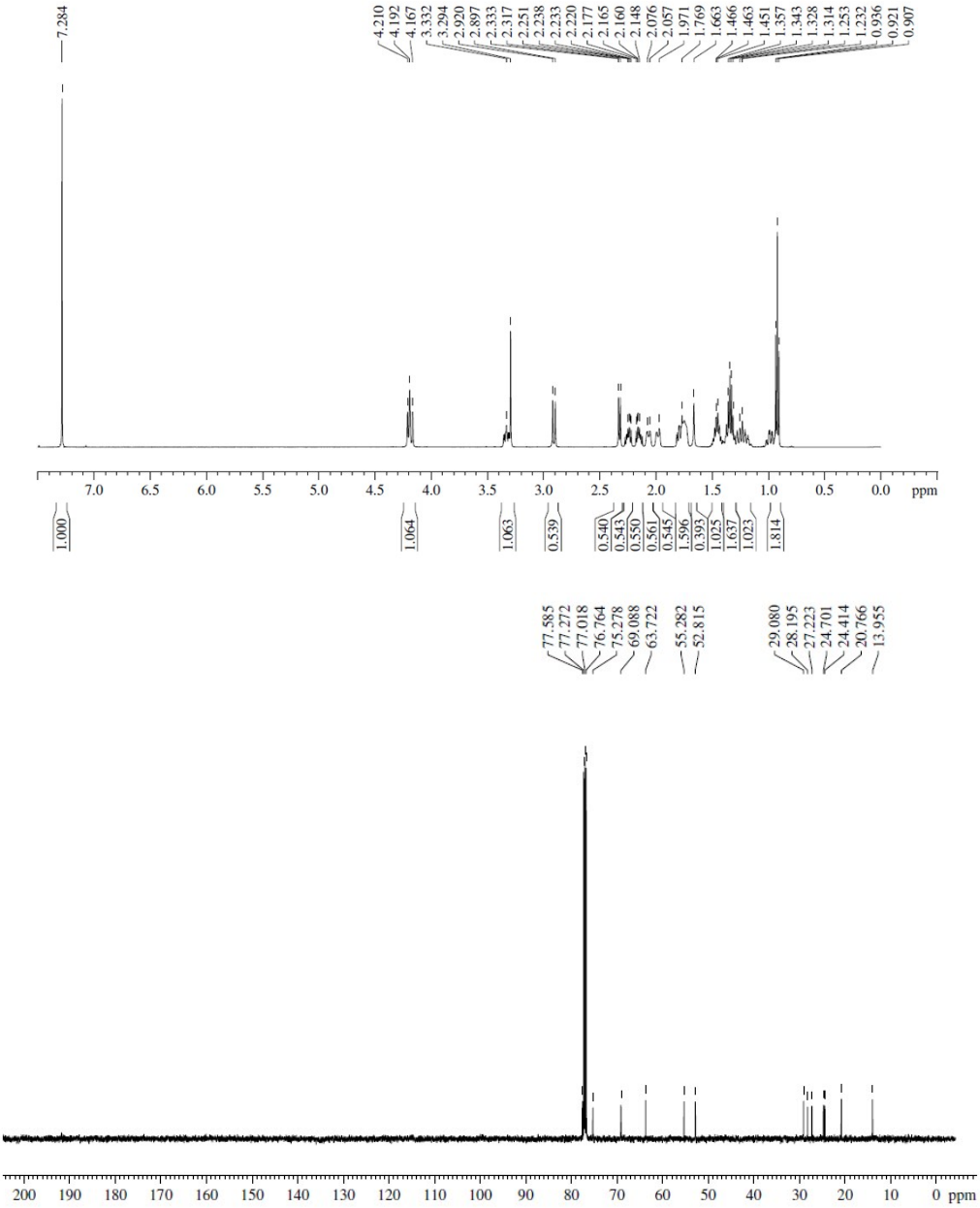
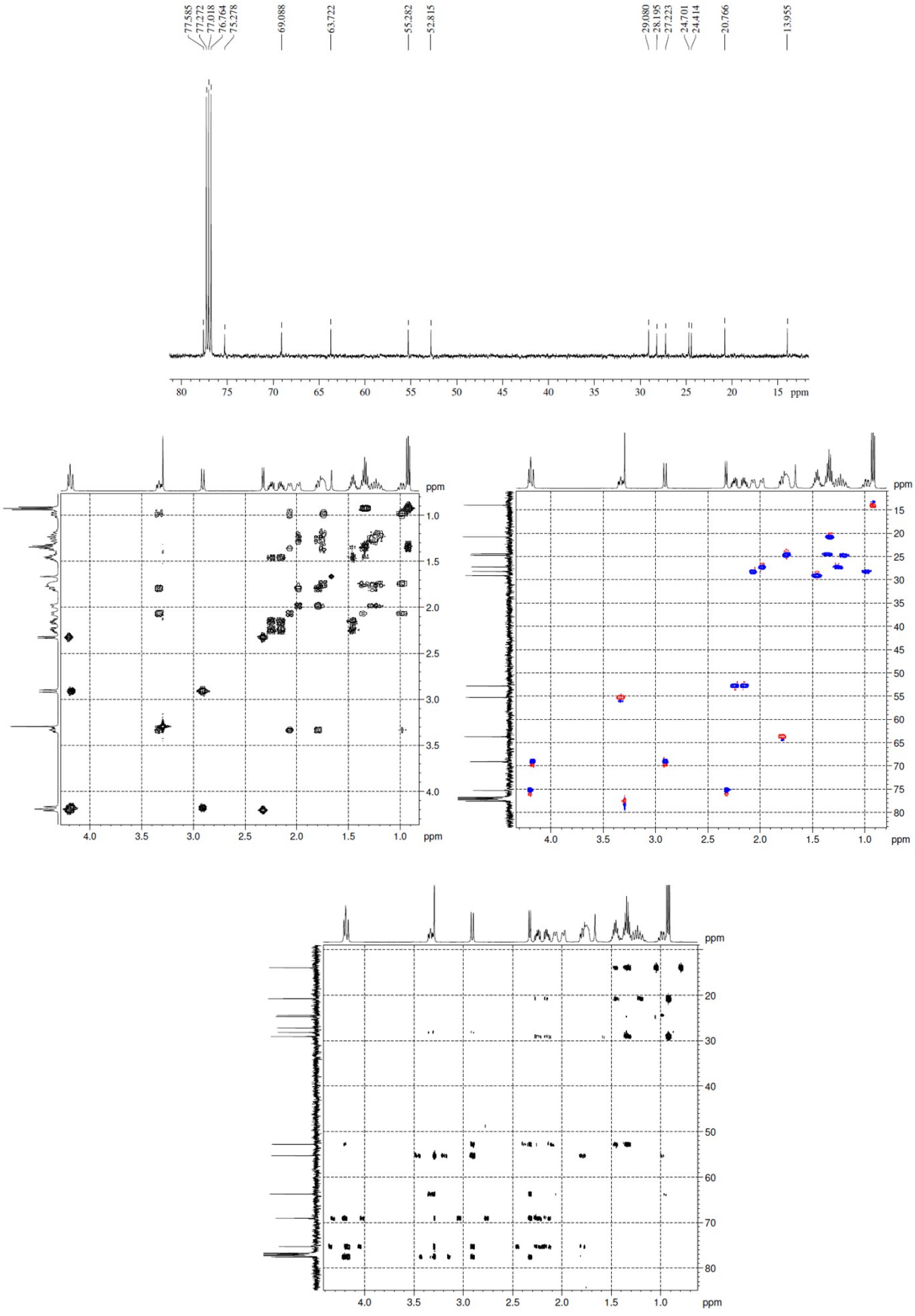


Figure 3. NMR spectra of compound **4**.




77.585
77.272
77.018
76.764
75.278
69.088
63.722
55.282
52.815
29.080
28.195
27.223
24.701
24.414
20.766
13.955
ppm

(3b*R**,7a*R**,10b*R**,14a*R**)-2,9-Di-*tert*-butyl-octadecahydro-1*H*,8*H*-2,3a,7b,9,10a,14b-hexaazadibenzo[*fg*,*op*]tetracene (**5**)

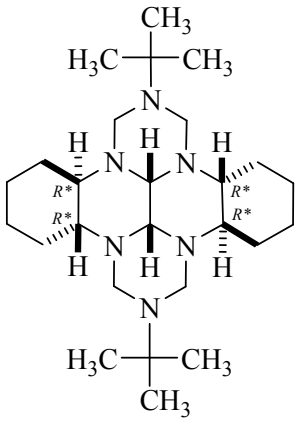
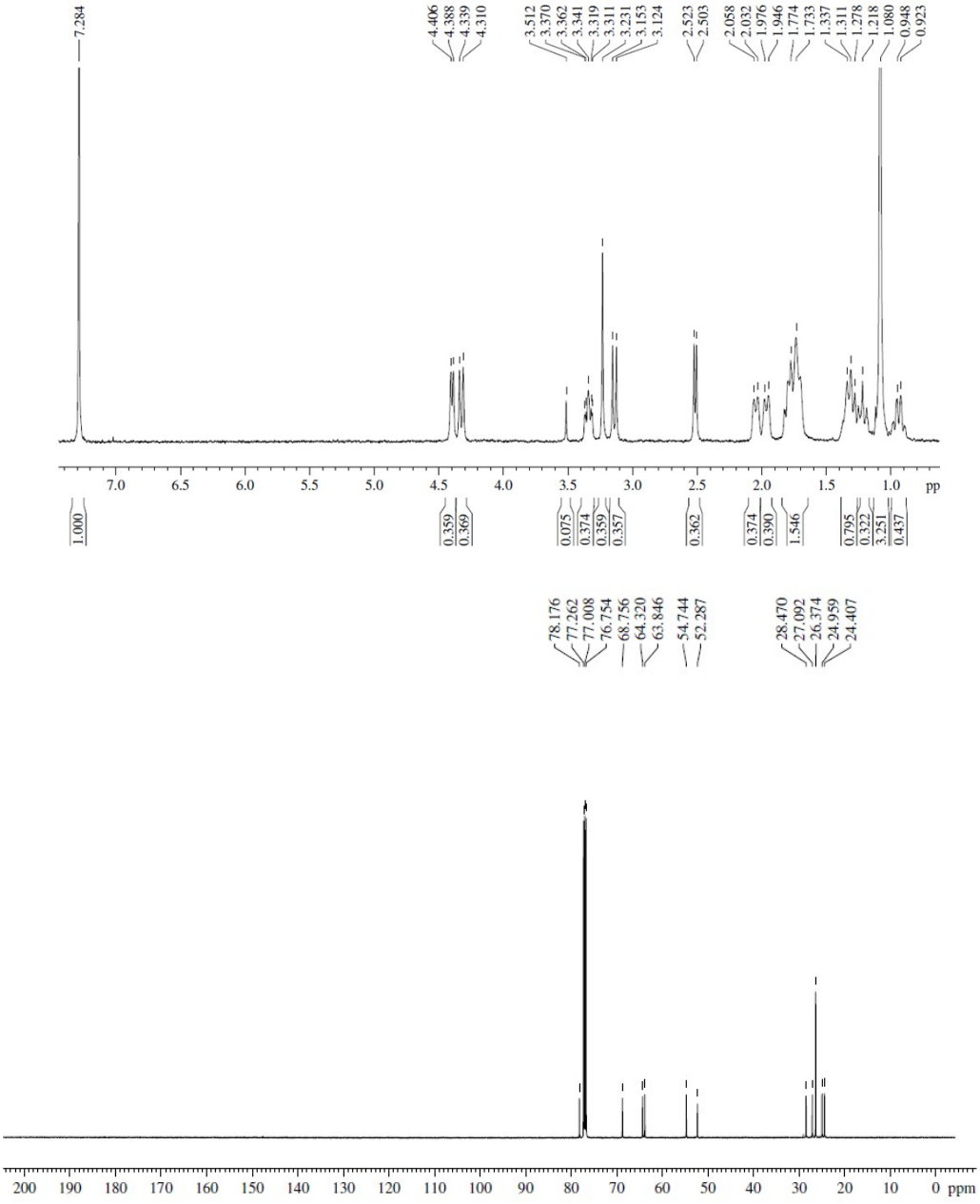
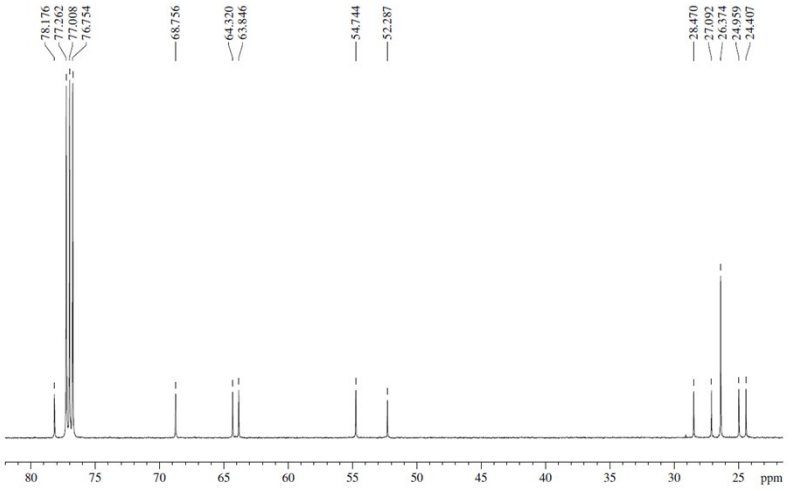
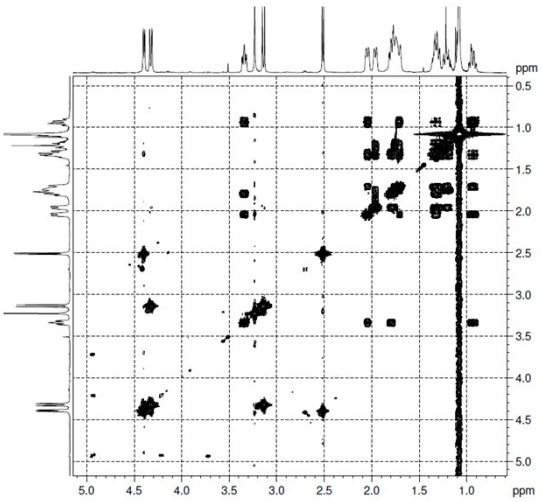
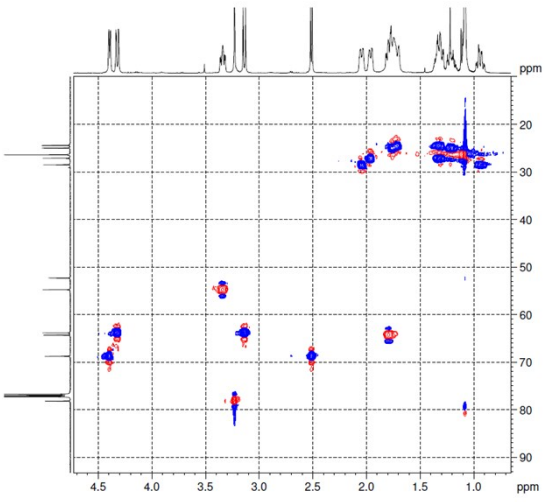


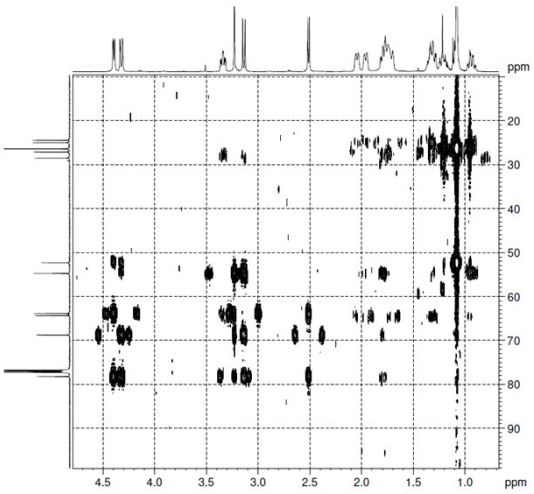
Figure 4. NMR and MS spectra of compound **5**.

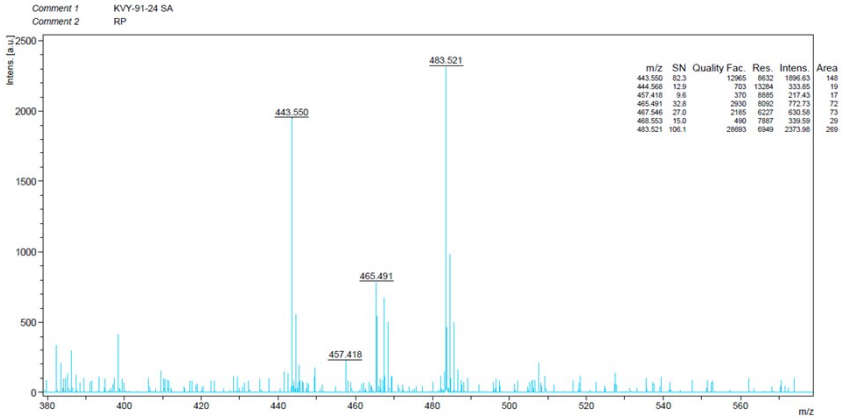



78.176
77.762
77.008
76.754
68.756
64.320
63.846
54.744
52.287
28.470
27.092
26.374
24.959
24.407
ppm


ppm


ppm


ppm


Comment 1 KVY-91-24 SA
Comment 2 RP
Intens. [a.u.]
m/z
483.521
443.550
465.491
457.418
m/z SN Quality Fac. Res. Intens. Area
443.550 82.3 12965 8632 1896.63 148
444.568 12.9 703 13284 333.85 19
457.418 9.6 370 8885 217.43 17
465.491 32.8 2930 8092 772.73 72
467.546 27.0 2185 6227 630.58 73
468.553 15.0 490 7887 339.59 29
483.521 106.1 26693 6949 2373.98 269

(3b*R**,7a*R**,10b*R**,14a*R**)-2,9-Dicyclopropyl-octadecahydro-1*H*,8*H*-2,3a,7b,9,10a,14b-hexaazadibenzo[*fg*,*op*]tetracene (**6**)

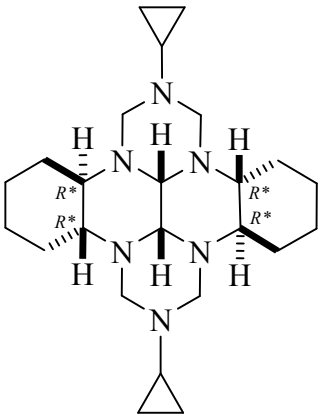
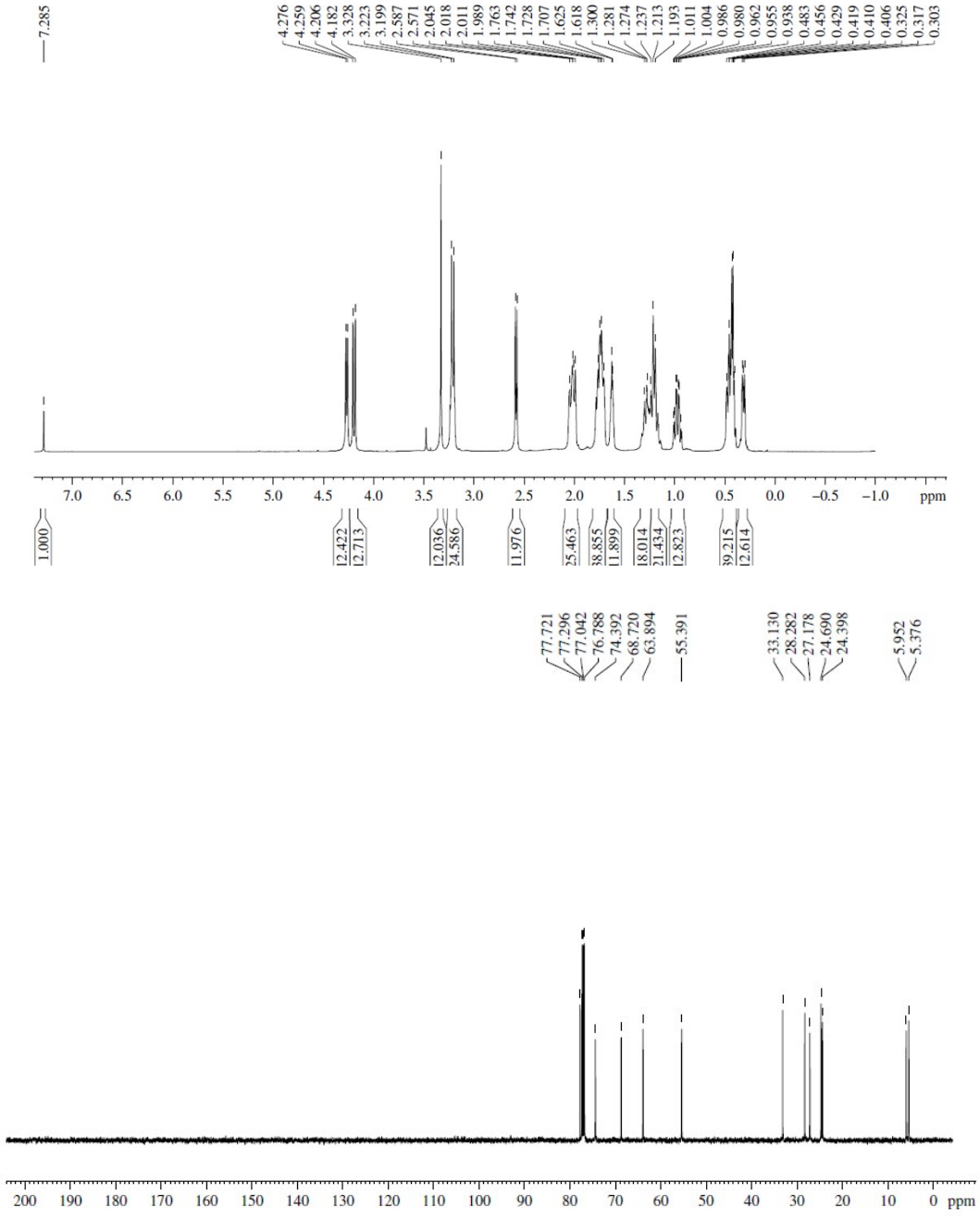
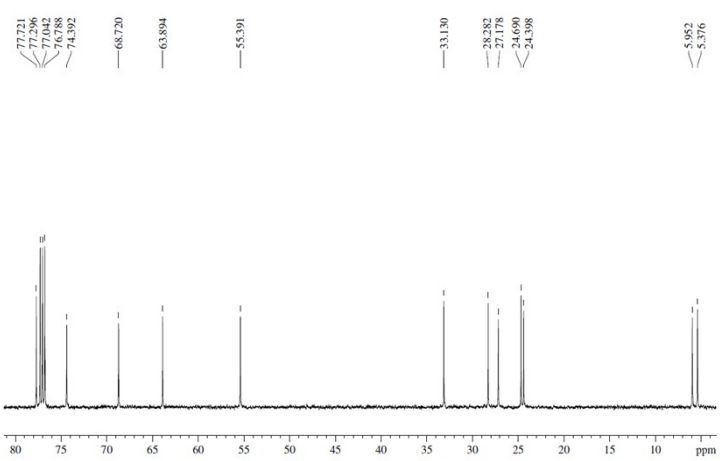
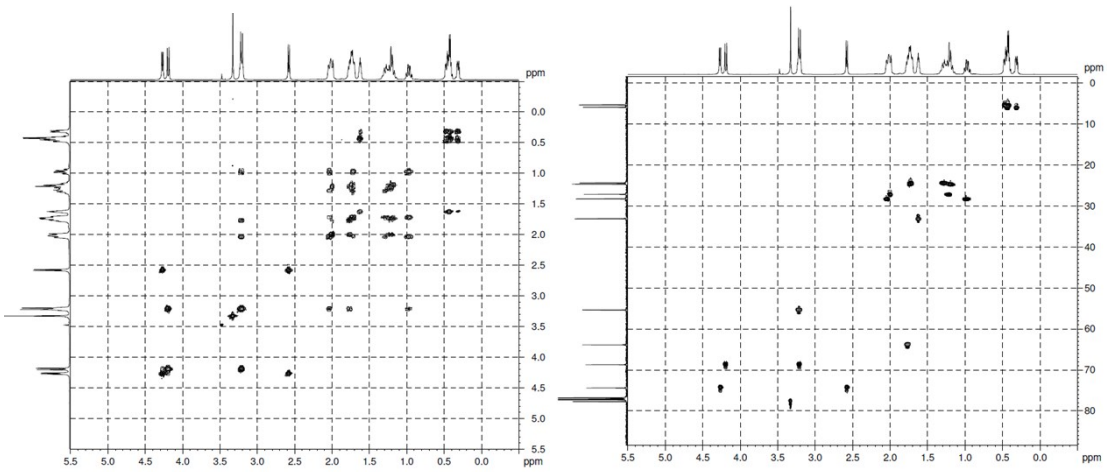


Figure 5. NMR and MS spectra of compound **6**.




77.721
77.396
77.042
76.788
74.392
68.720
63.894
55.391
33.130
28.282
27.178
24.690
24.398
5.952
5.376
80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 ppm


ppm
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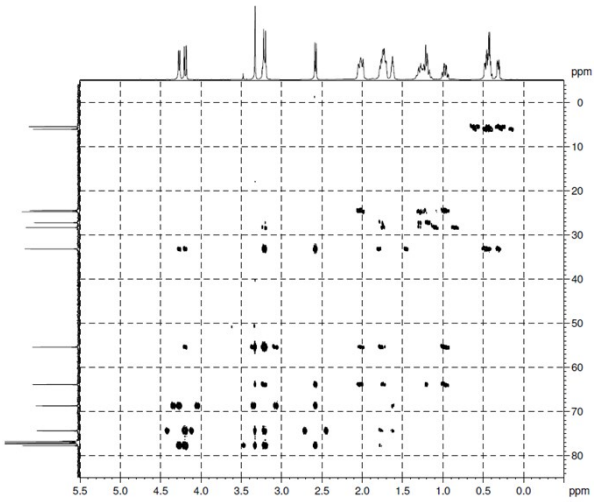
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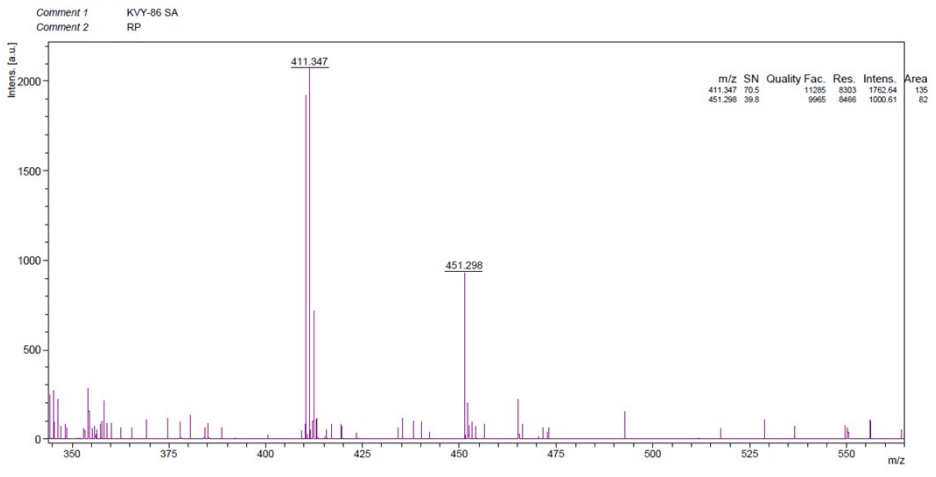
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Comment 2 RP
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411.347
451.298
m/z SN Quality Fac. Res. Intens. Area
411.347 70.5 11285 8303 1762.64 135
451.298 39.8 9965 8466 1000.61 82
350 375 400 425 450 475 500 525 550 m/z

(3b*R**,7a*R**,10b*R**,14a*R**)-2,9-Dicyclopenthyl-octadecahydro-1*H*,8*H*-2,3a,7b,9,10a,14b-hexaazadibenzo[*fg*,*op*]tetracene (**7**)

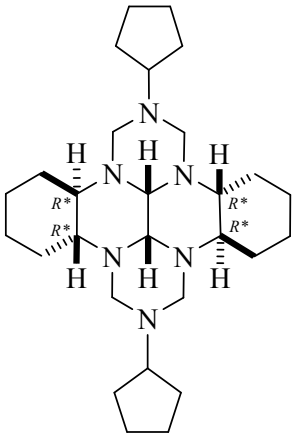
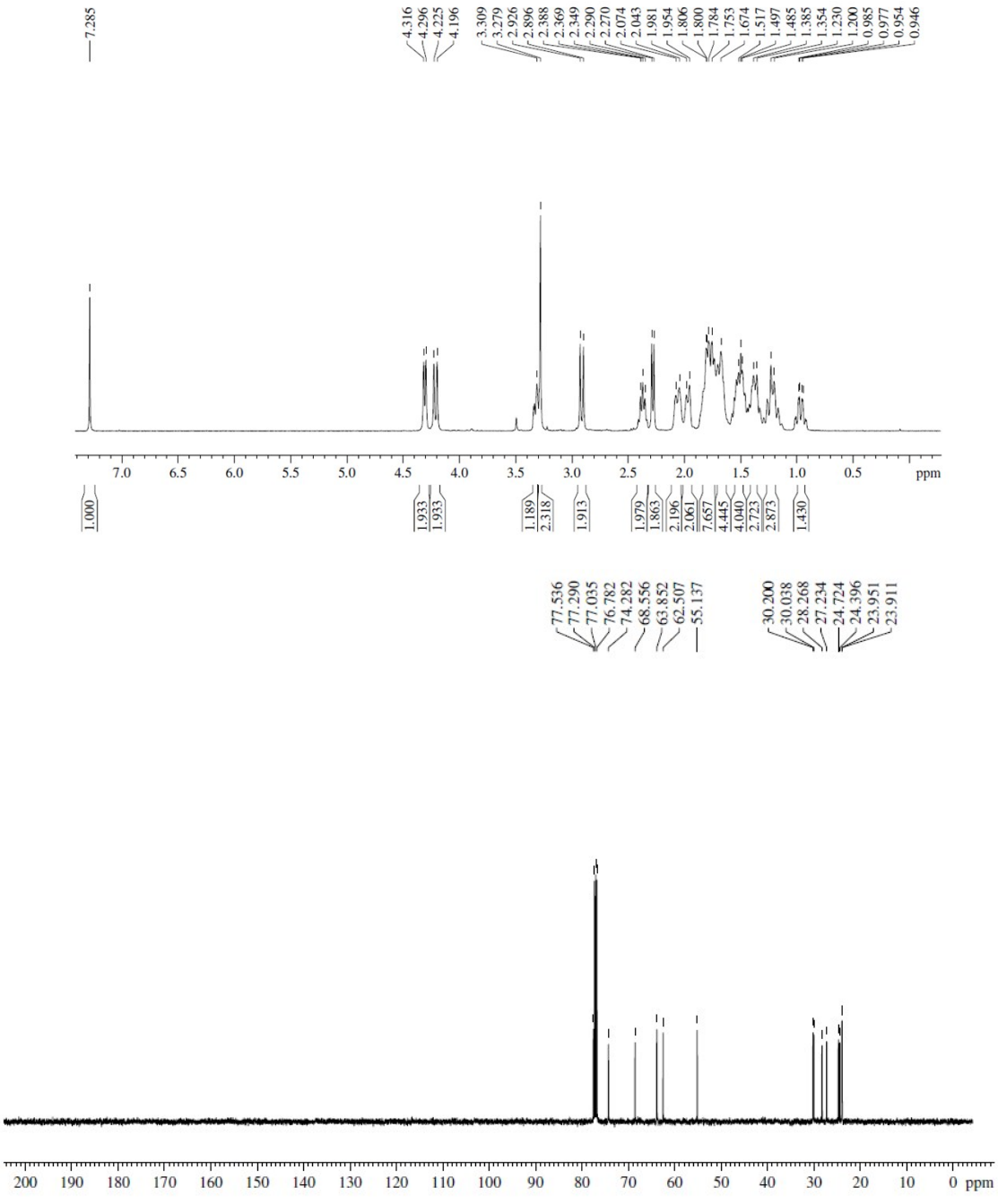
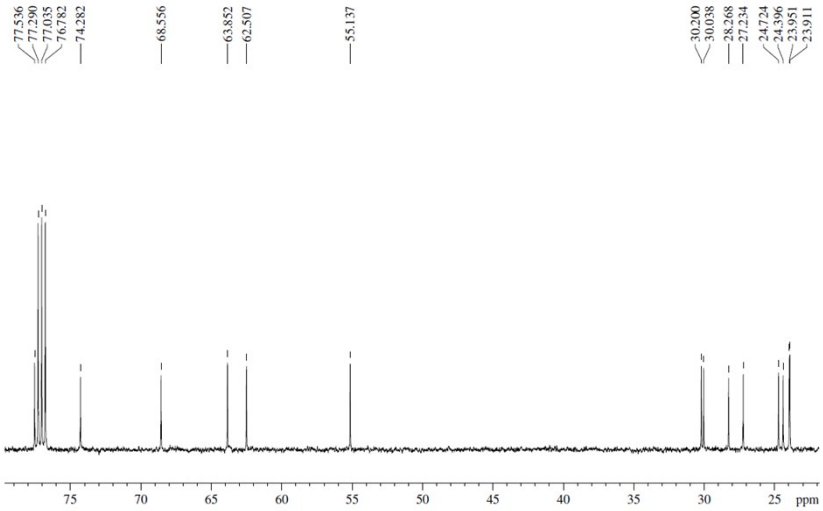
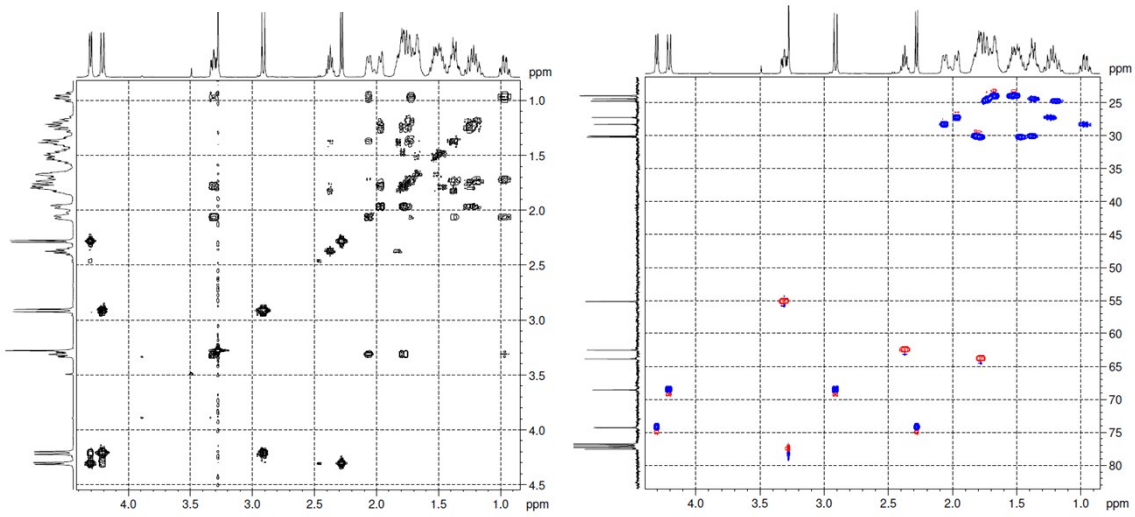
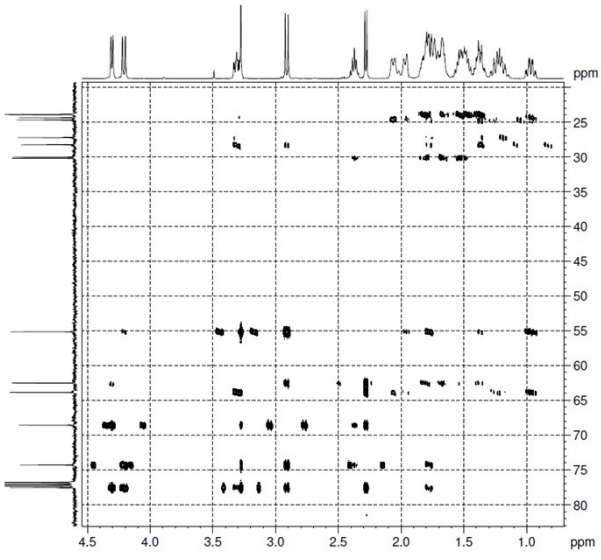


Figure 6. NMR spectra of compound **7**.




77.536
77.290
77.035
76.782
74.282
68.556
63.852
62.507
55.137
30.200
30.038
28.268
27.234
24.724
24.396
23.951
23.911
75
70
65
60
55
50
45
40
35
30
25
ppm


ppm
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
ppm
25
30
35
40
45
50
55
60
65
70
75
80
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm


ppm
25
30
35
40
45
50
55
60
65
70
75
80
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm

(3b*R**,7a*R**,10b*R**,14a*R**)-2,9-Dicyclohexyl-octadecahydro-1*H*,8*H*-2,3a,7b,9,10a,14b-hexaazadibenzo[*fg*,*op*]tetracene (**8**)

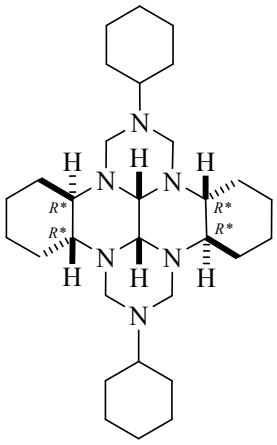
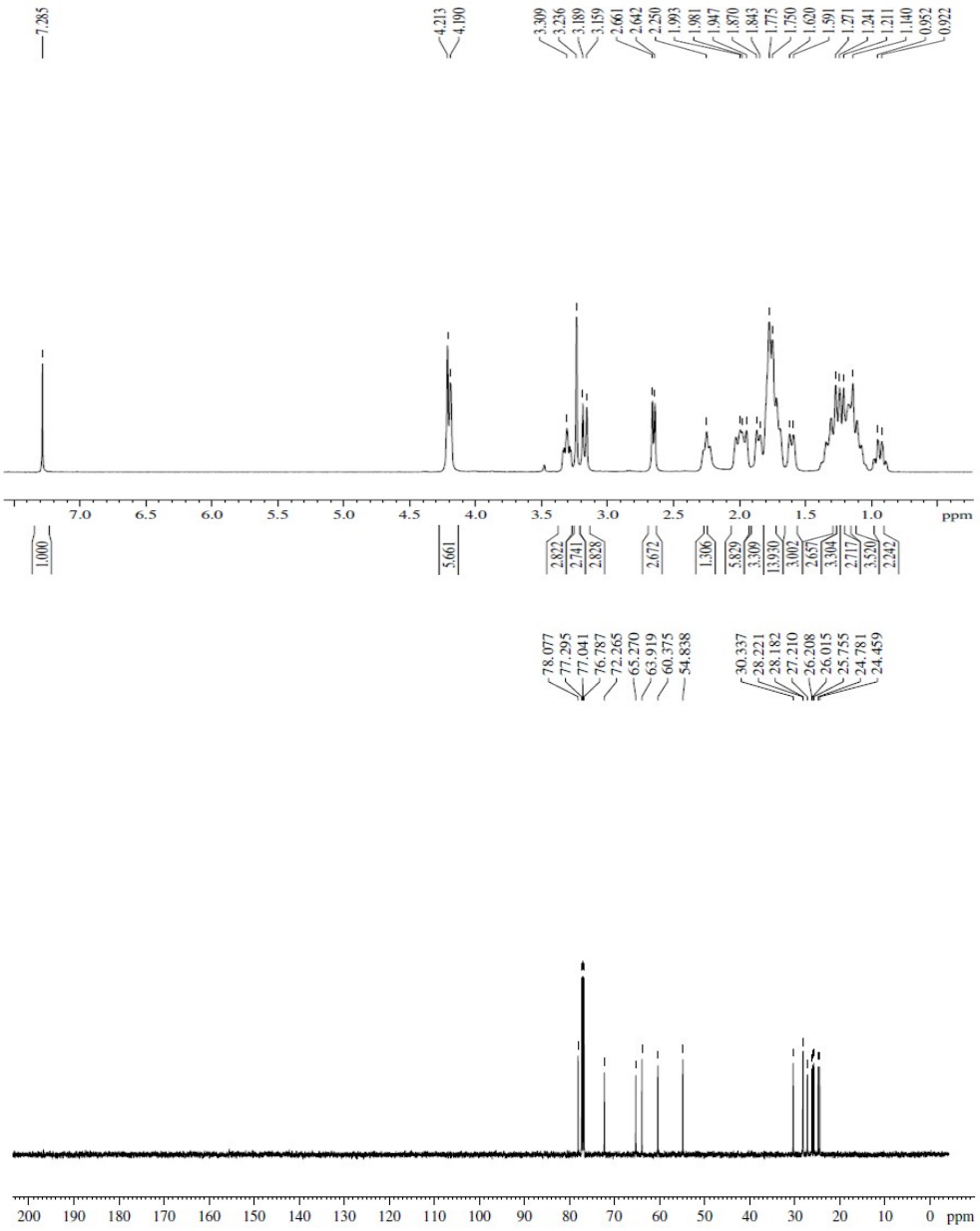
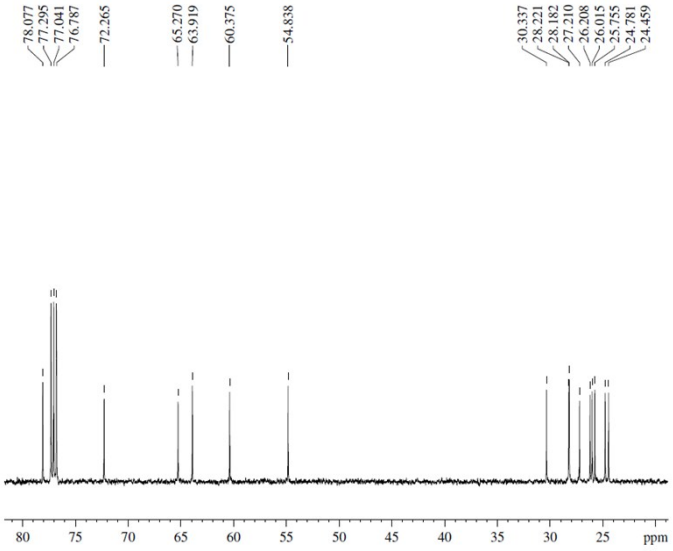
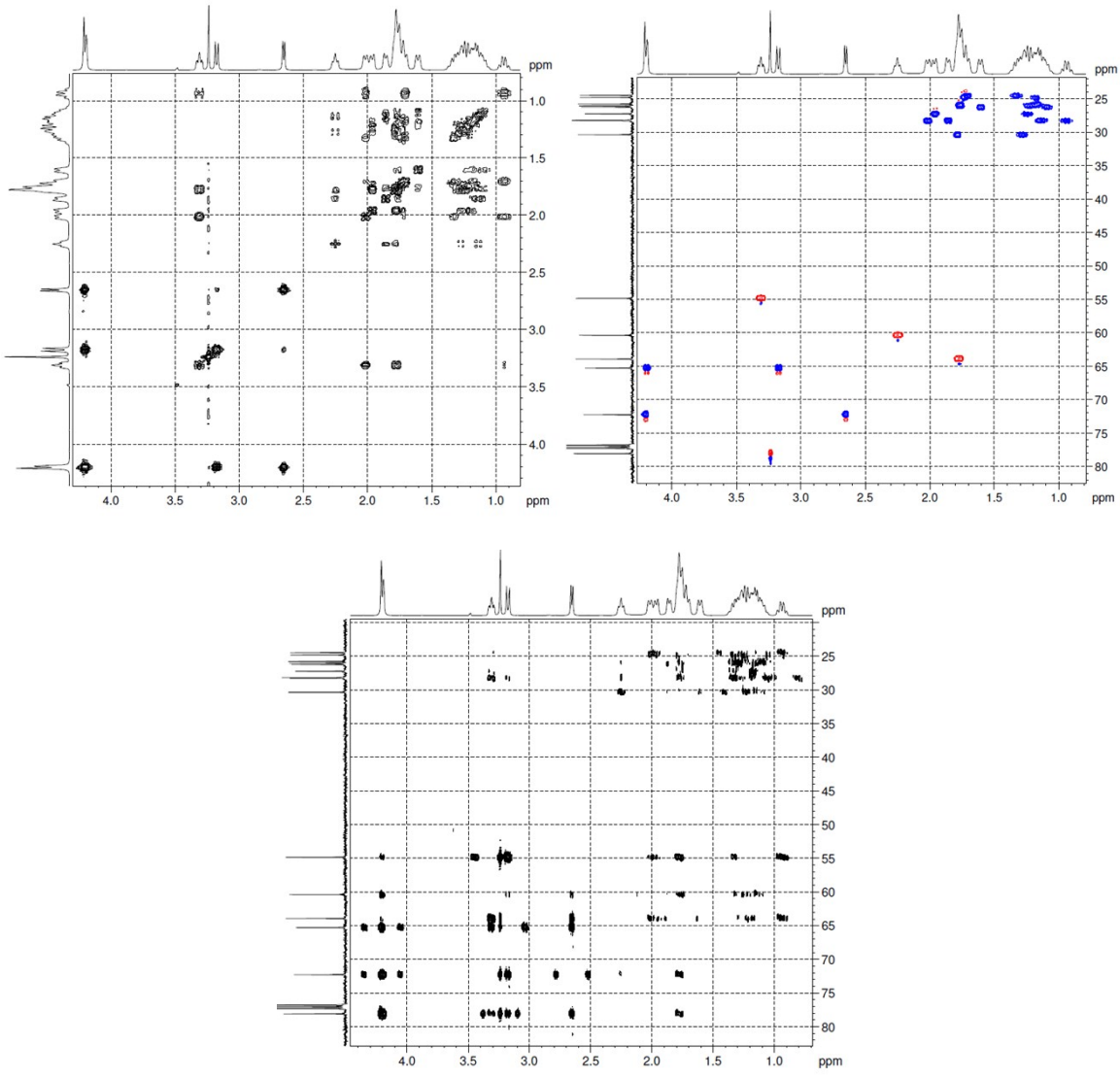


Figure 7. NMR spectra of compound **8**.




78.077
77.295
77.041
76.787
72.265
65.270
63.919
60.375
54.838
30.337
28.221
28.182
27.210
26.208
26.015
25.755
24.781
24.459
80 75 70 65 60 55 50 45 40 35 30 25 ppm


ppm
1.0 1.5 2.0 2.5 3.0 3.5 4.0
4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
ppm
25 30 35 40 45 50 55 60 65 70 75 80
4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
ppm
25 30 35 40 45 50 55 60 65 70 75 80
4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm

(3b*R**,7a*R**,10b*R**,14a*R**)-2,9-Dicycloheptyl-octadecahydro-1*H*,8*H*-2,3a,7b,9,10a,14b-hexaazadibenzo[*fg*,*op*]tetracene (**9**)

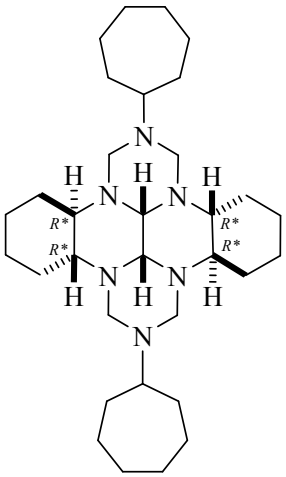
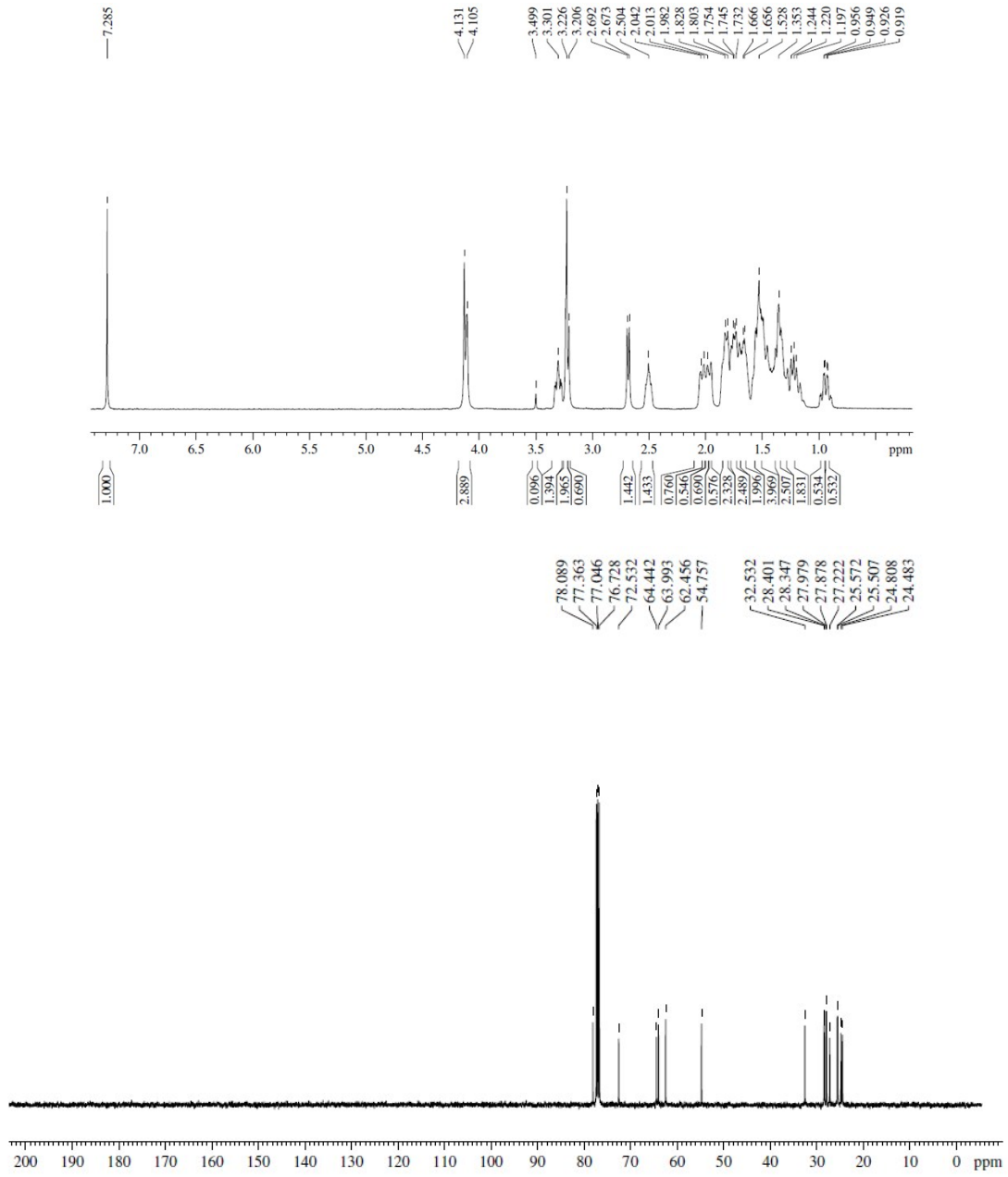
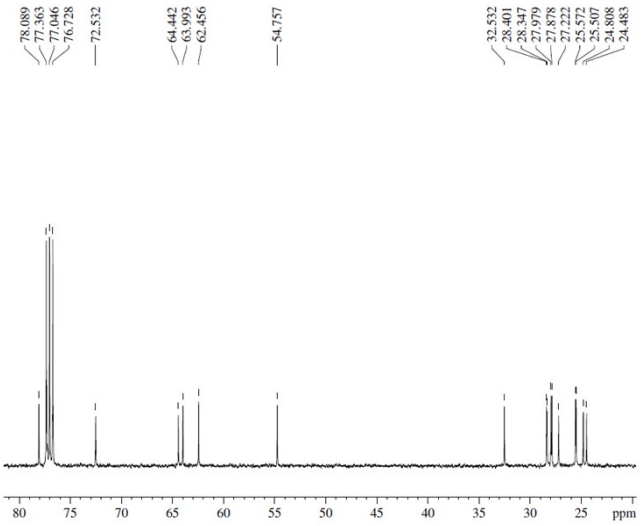
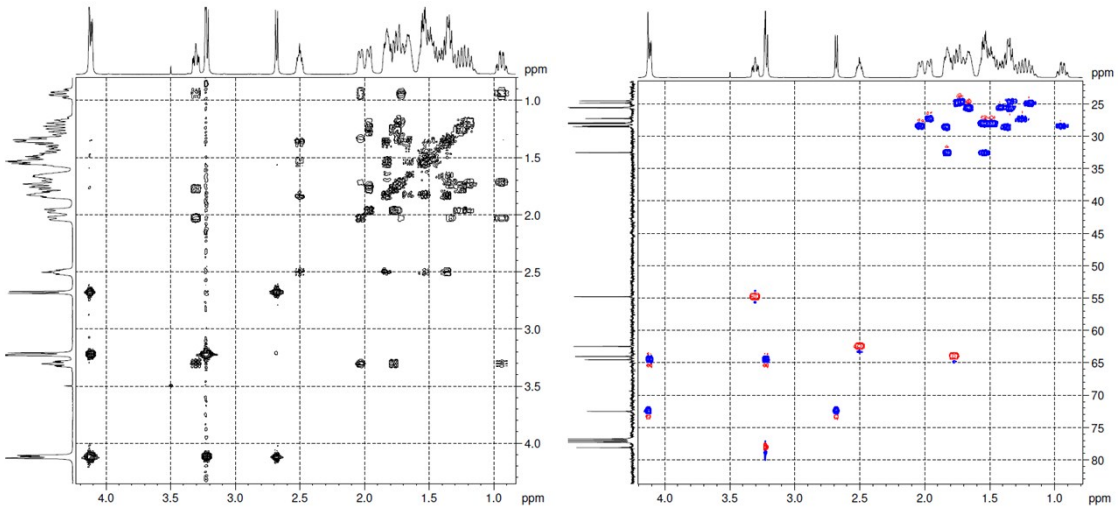
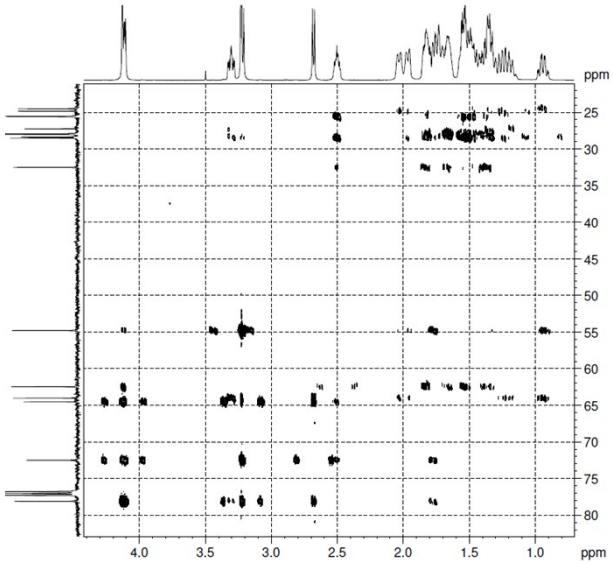


Figure 8. NMR spectra of compound **9**.




78.089
77.363
77.046
76.728
72.532
64.442
63.993
62.456
54.757
32.532
28.401
28.347
27.979
27.878
27.222
25.572
25.507
24.808
24.483
80 75 70 65 60 55 50 45 40 35 30 25 ppm


ppm
4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
ppm
4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm


ppm
4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm

(3b*R**,7a*R**,10b*R**,14a*R**)-2,9-Dicyclooctyl-octadecahydro-1*H*,8*H*-2,3a,7b,9,10a,14b-hexaazadibenzo[*fg*,*op*]tetracene (**10**)

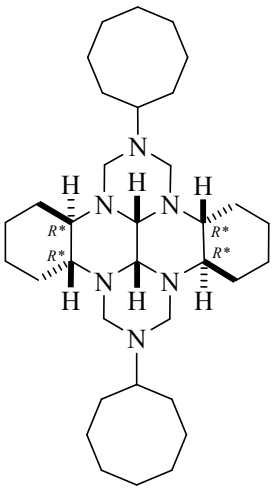
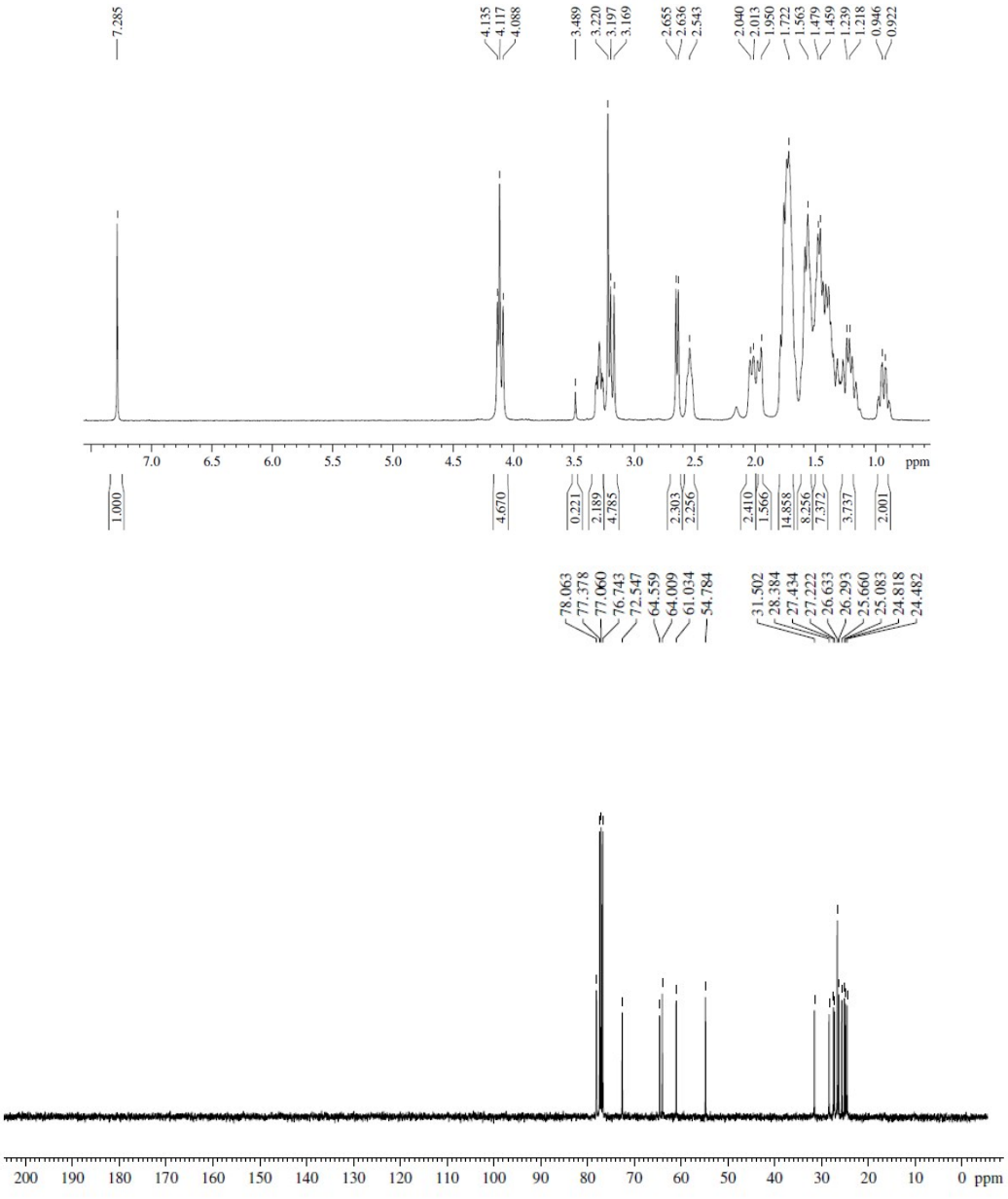
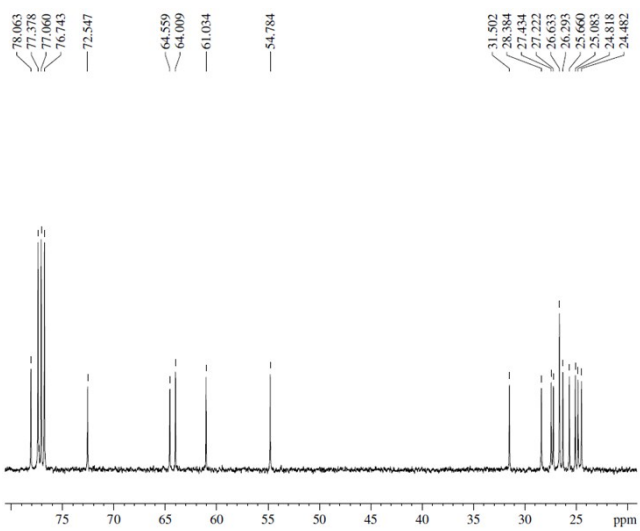
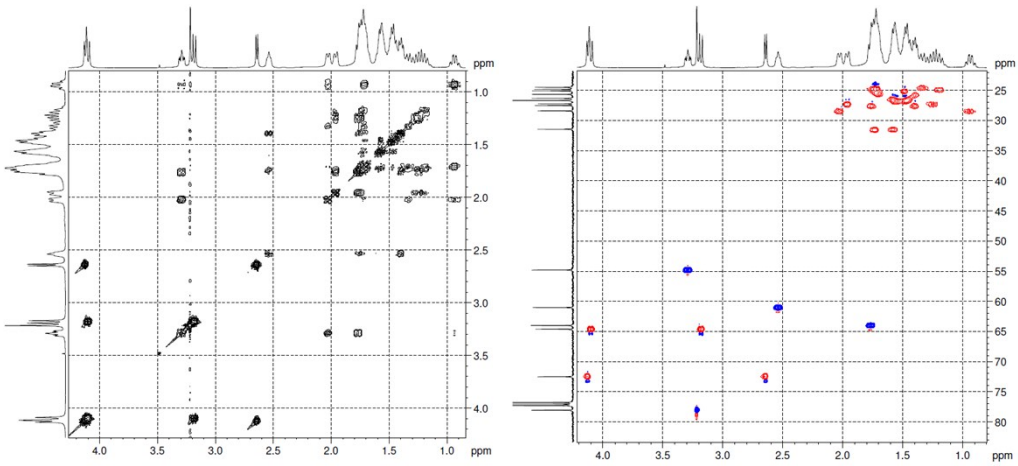
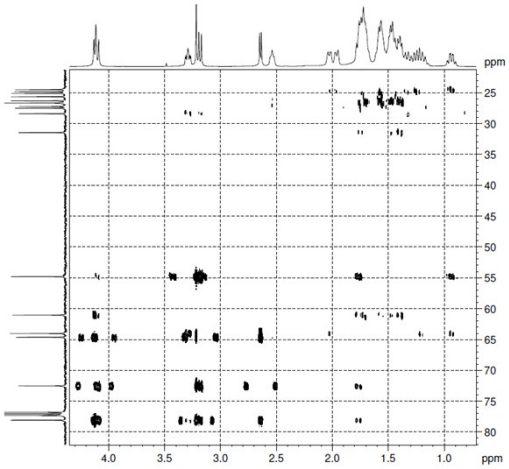


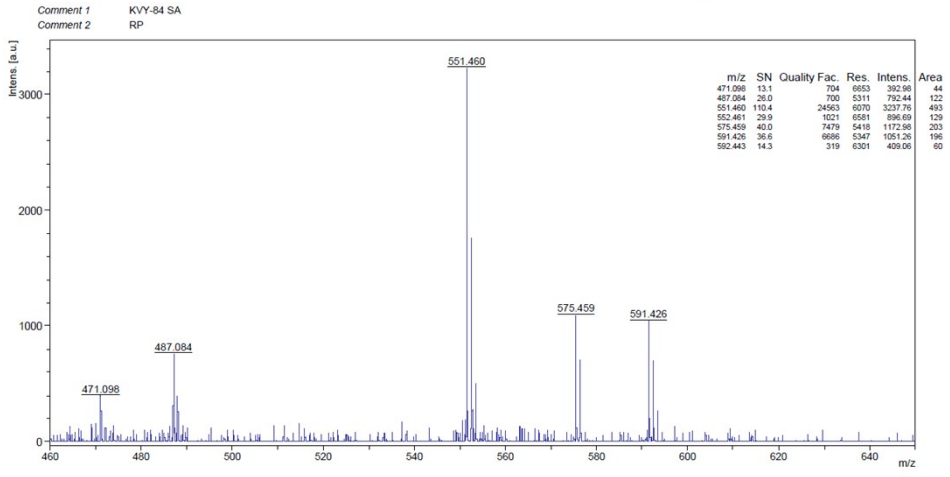
Figure 9. NMR and MS spectra of compound **10**.




78.063
77.378
77.060
76.743
72.547
64.559
64.009
61.034
54.784
31.502
28.384
27.434
27.222
26.633
26.293
25.660
25.083
24.818
24.482
75 70 65 60 55 50 45 40 35 30 25 ppm


ppm
4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
ppm
4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm


ppm
4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm


Comment 1 KVY-84 SA
Comment 2 RP
Intens. [a.u.]
551.460
575.459
591.426
487.084
471.098
m/z SN Quality Fac. Res. Intens. Area
471.098 13.1 704 6653 392.98 44
487.084 26.0 700 5311 792.44 122
551.460 110.4 24563 6070 3237.76 493
552.461 29.9 1021 6581 896.69 129
575.459 40.0 7479 5418 1172.98 203
591.426 36.6 6686 5347 1051.26 196
592.443 14.3 319 6301 409.06 60
460 480 500 520 540 560 580 600 620 640 m/z

(3b*R**,7a*R**,10b*R**,14a*R**)-2,9-Dibicyclo[2.2.1]hept-2-yl-octadecahydro-1*H*,8*H*-2,3a,7b,9,10a,14b-hexaazadibenzo[*fg*,*op*]tetracene (**11**)

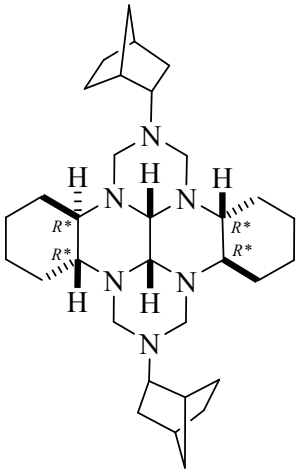
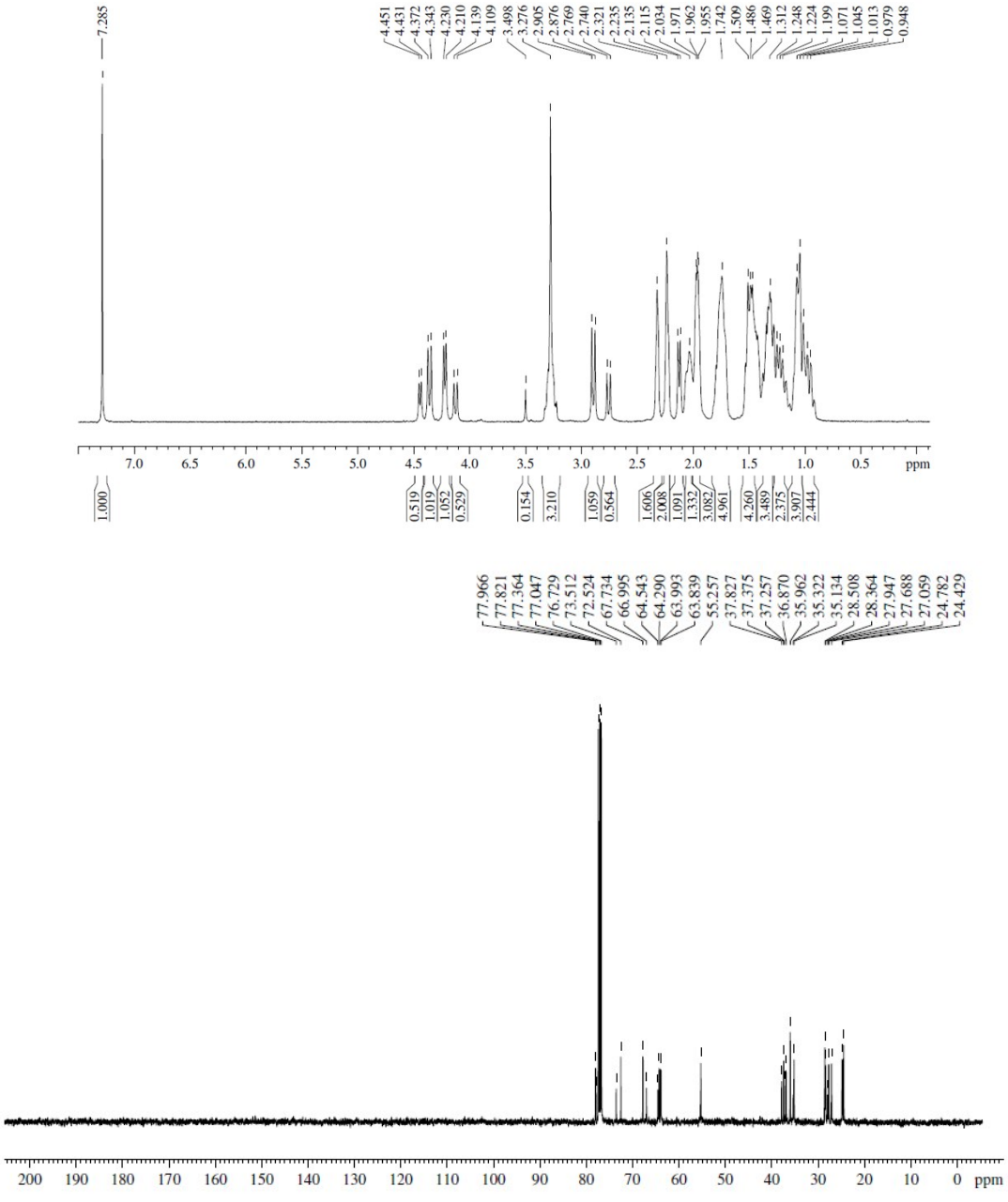
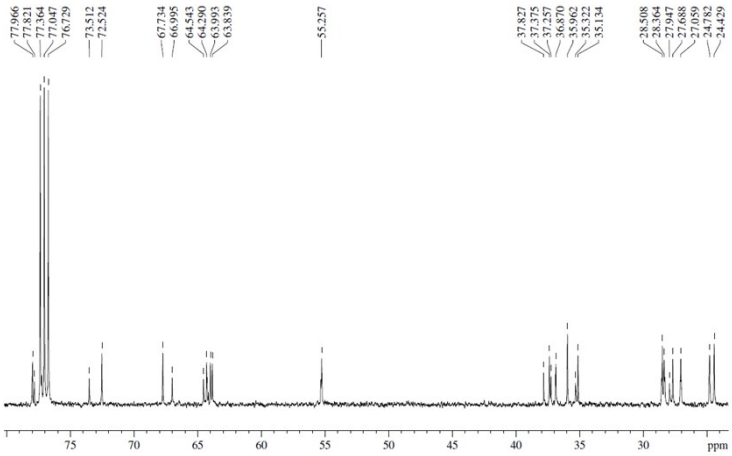
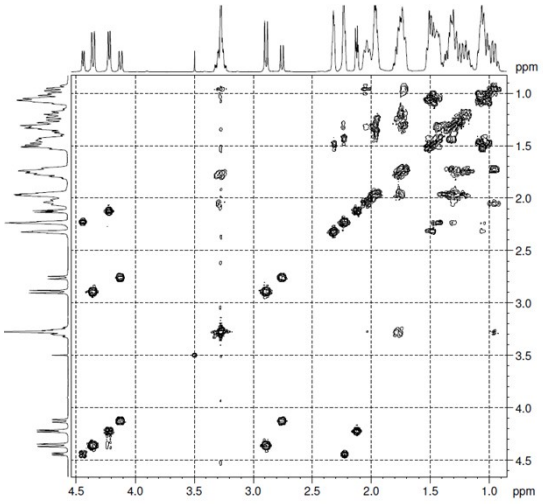
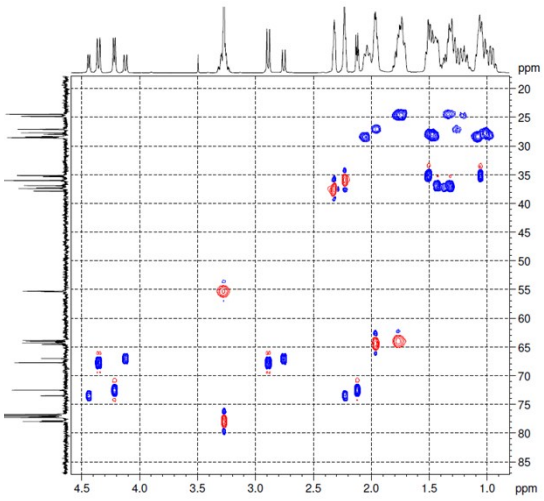


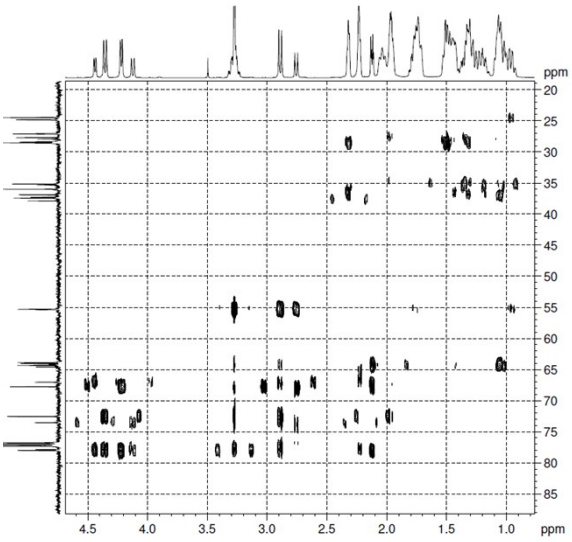
Figure 10. NMR spectra of compound **11**.




77.966
77.821
77.464
77.047
76.729
73.512
72.524
67.734
66.995
64.543
64.290
63.993
63.839
55.257
37.827
37.375
37.257
36.870
36.662
35.522
35.134
28.508
28.364
27.947
27.688
27.059
24.782
24.429
75
70
65
60
55
50
45
40
35
30
ppm


ppm
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm


ppm
20
25
30
35
40
45
50
55
60
65
70
75
80
85
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm


ppm
20
25
30
35
40
45
50
55
60
65
70
75
80
85
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm

(3b*R**,7a*R**,10b*R**,14a*R**)-2,9-Di(1-adamantyl)-octadecahydro-1*H*,8*H*-2,3a,7b,9,10a,14b-hexaazadibenzo[*fg*,*op*]tetracene (**12**)

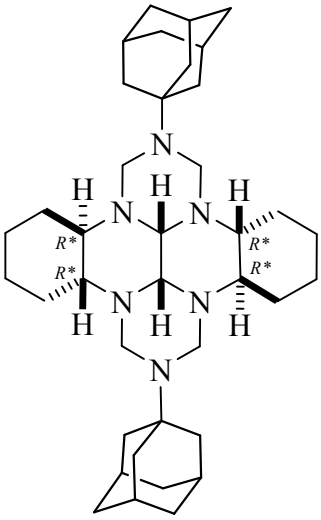
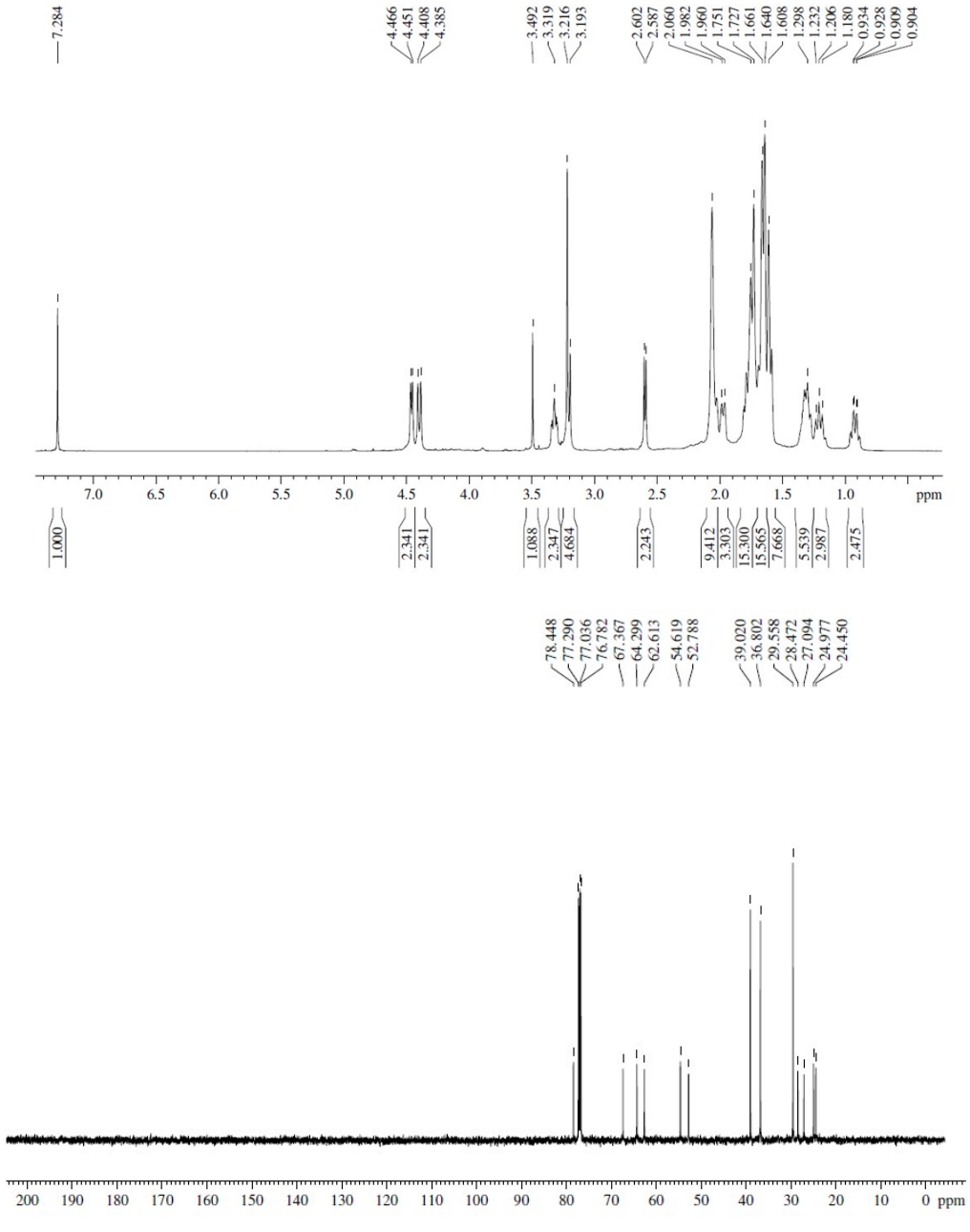
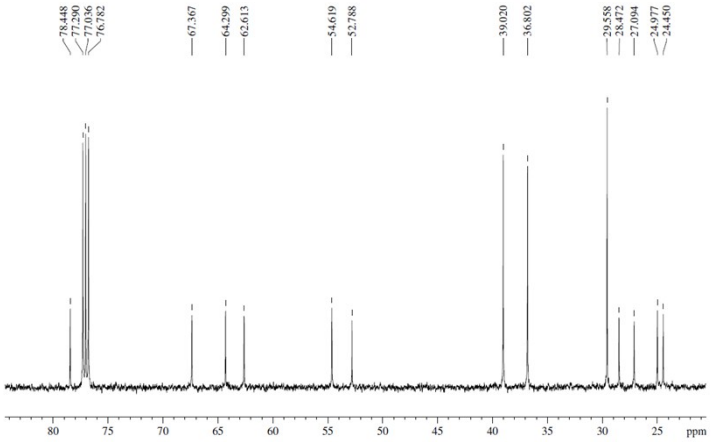
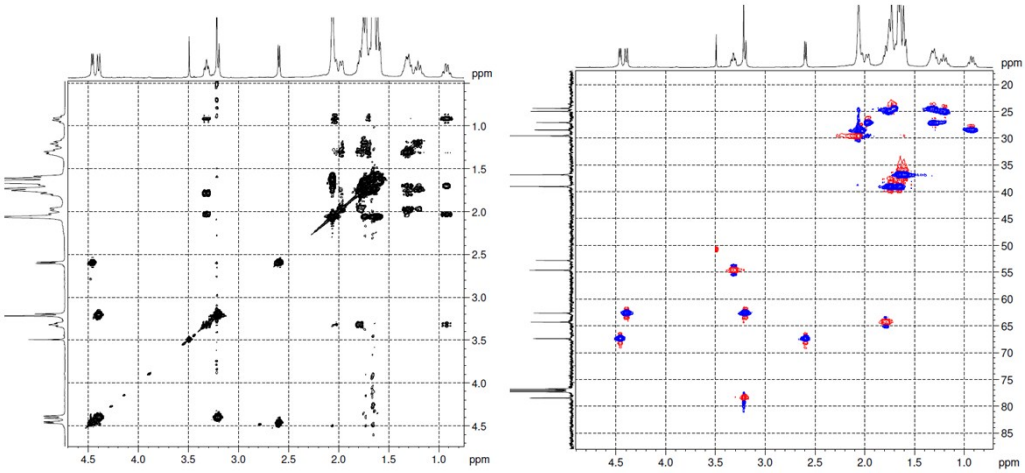
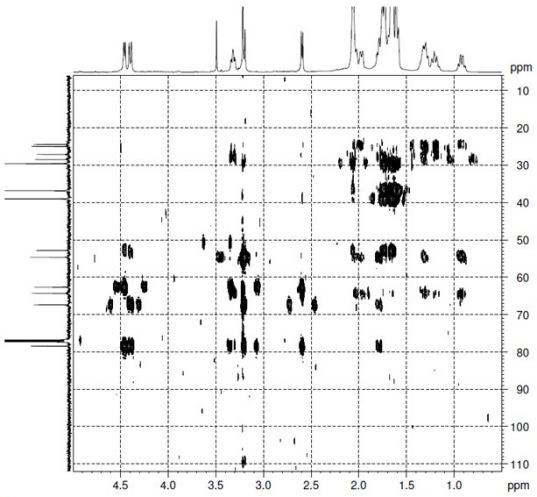


Figure 11. NMR and MS spectra of compound **12**.

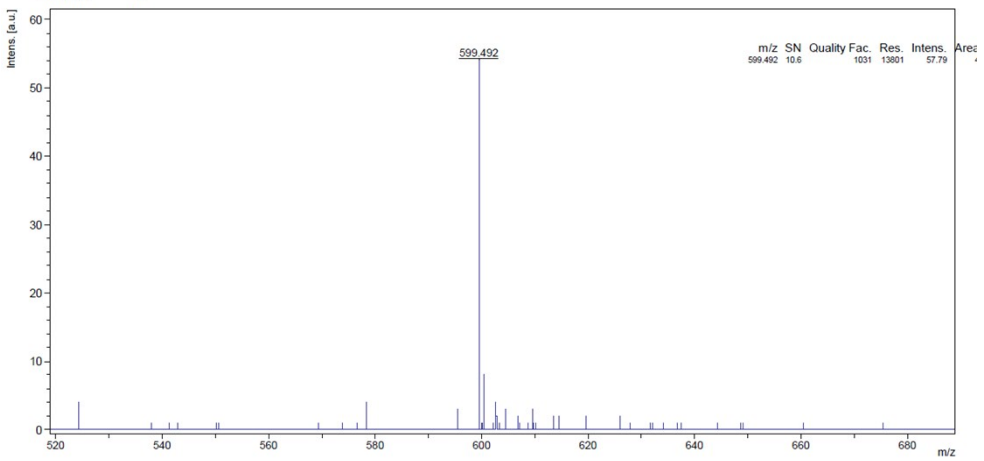








Comment 1 KVY-120 sinapic acid
Comment 2 RP



(3b*R**,7a*R**,10b*R**,14a*R**)-2,9-Di(2-adamantyl)-octadecahydro-1*H*,8*H*-2,3a,7b,9,10a,14b-hexaazadibenzo[*fg*,*op*]tetracene (**13**)

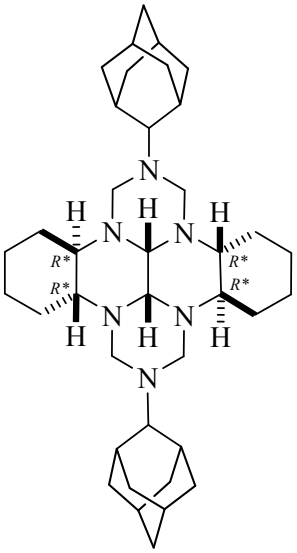
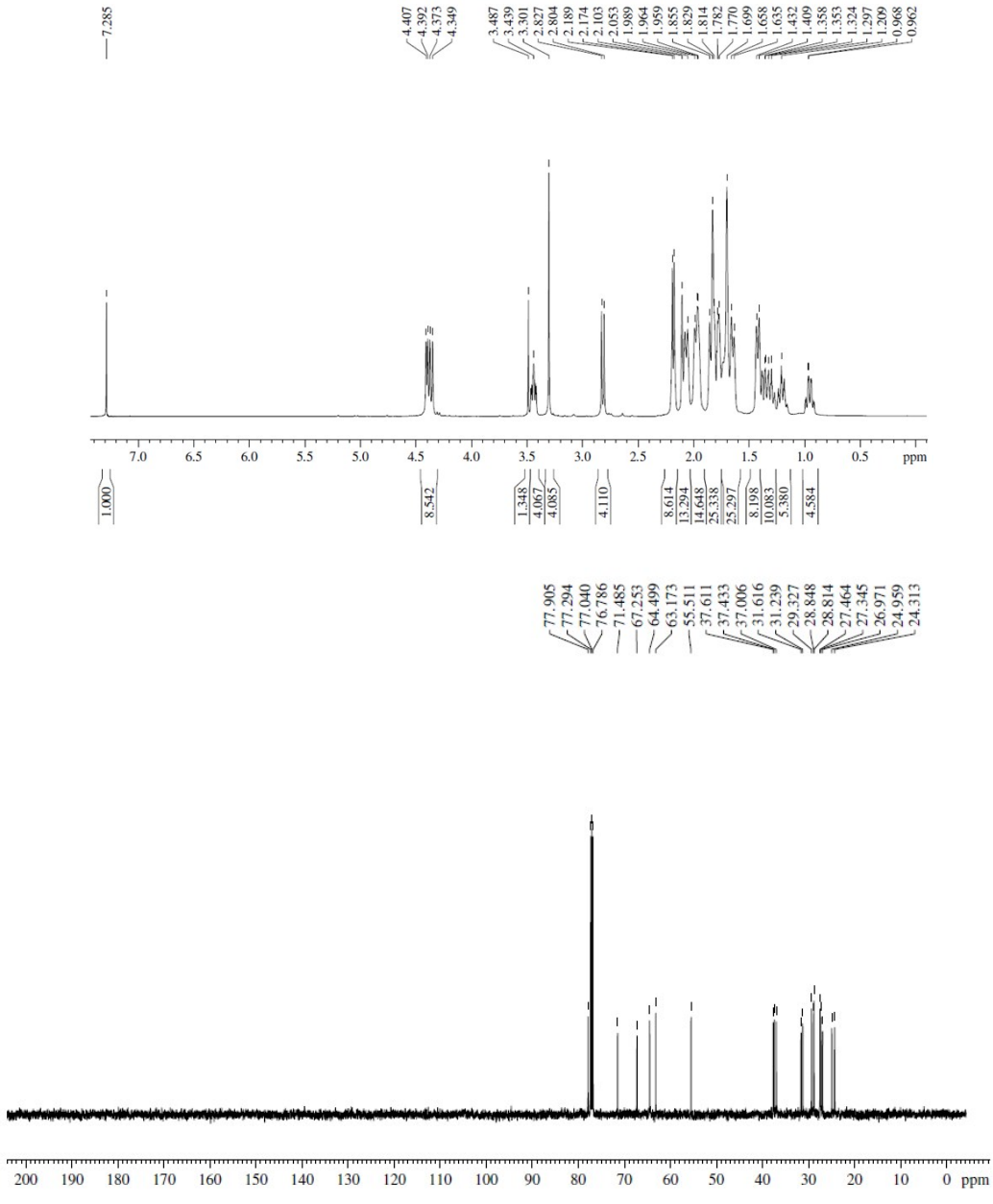
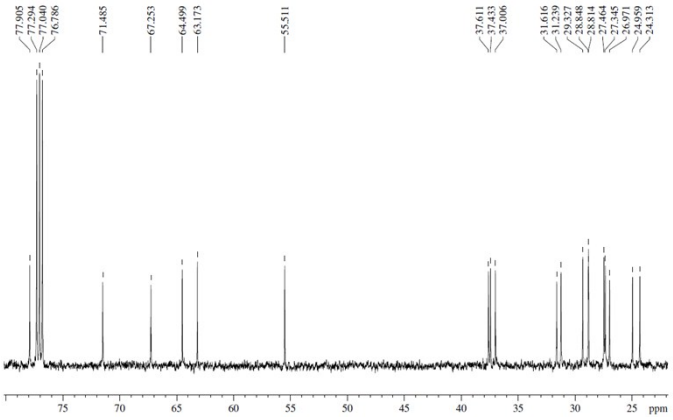
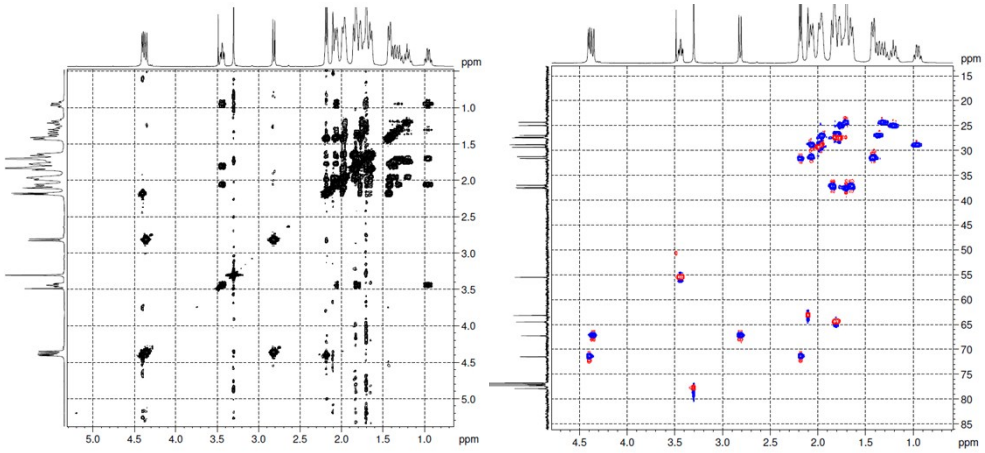
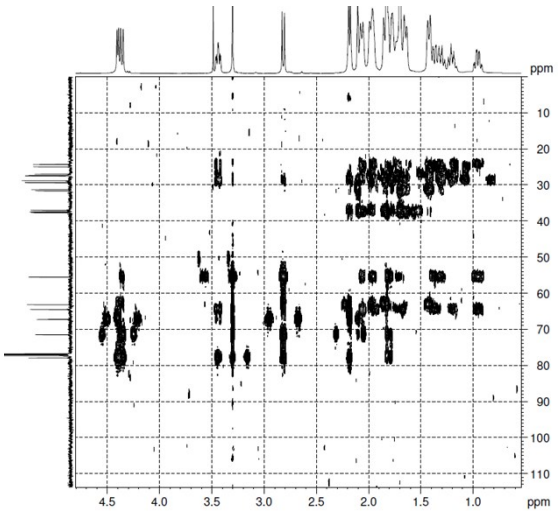


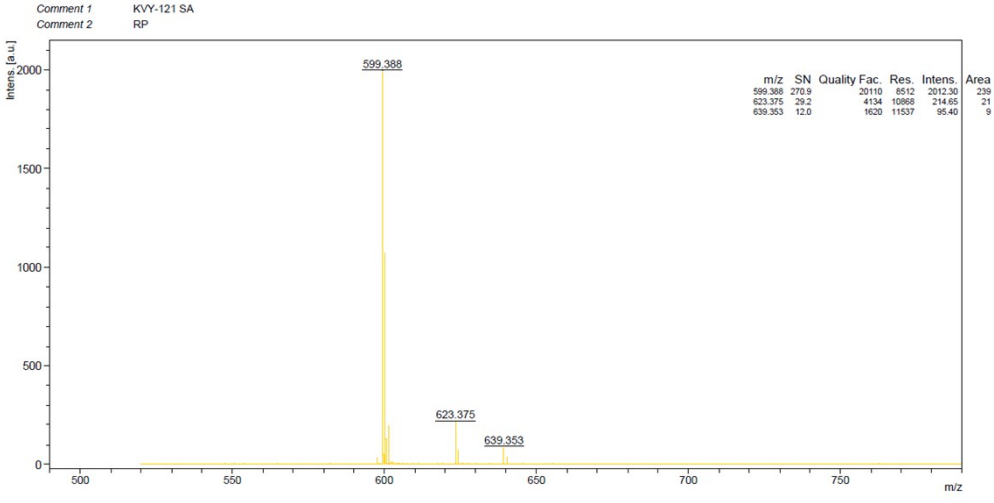
Figure 12. NMR and MS spectra of compound **13**.




77.905
77.294
77.040
76.786
71.485
67.253
64.499
63.173
55.511
37.611
37.433
37.006
31.616
31.239
29.327
28.848
28.814
27.464
27.345
26.971
24.959
24.313
ppm


ppm
ppm


ppm
ppm


Comment 1 KVY-121 SA
Comment 2 RP
Intens. [a.u.]
599.388
623.375
639.353
m/z SN Quality Fac. Res. Intens. Area
599.388 270.9 20110 8512 2012.30 239
623.375 29.2 4134 10868 214.65 21
639.353 12.0 1620 11537 95.40 9
m/z

(3b*R**,7a*R**,10b*R**,14a*R**)-2,9-Bis(1-hydroxy-3-adamantyl)-octadecahydro-1*H*,8*H*-2,3a,7b,9,10a,14b-hexaazadibenzo[*fg*,*op*]tetracene (**14**)

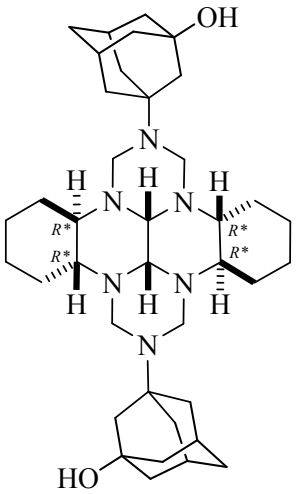
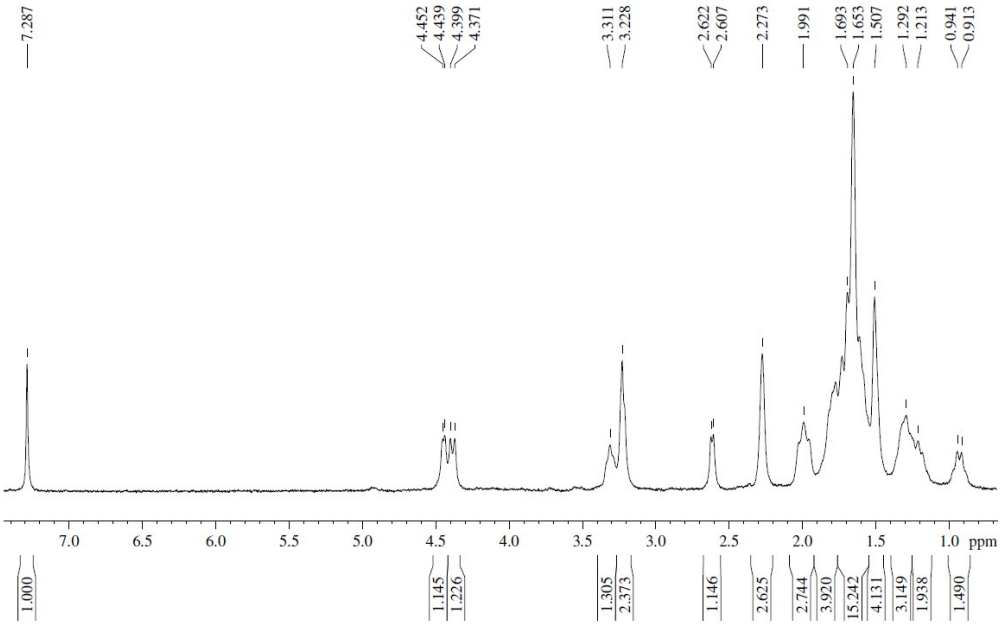
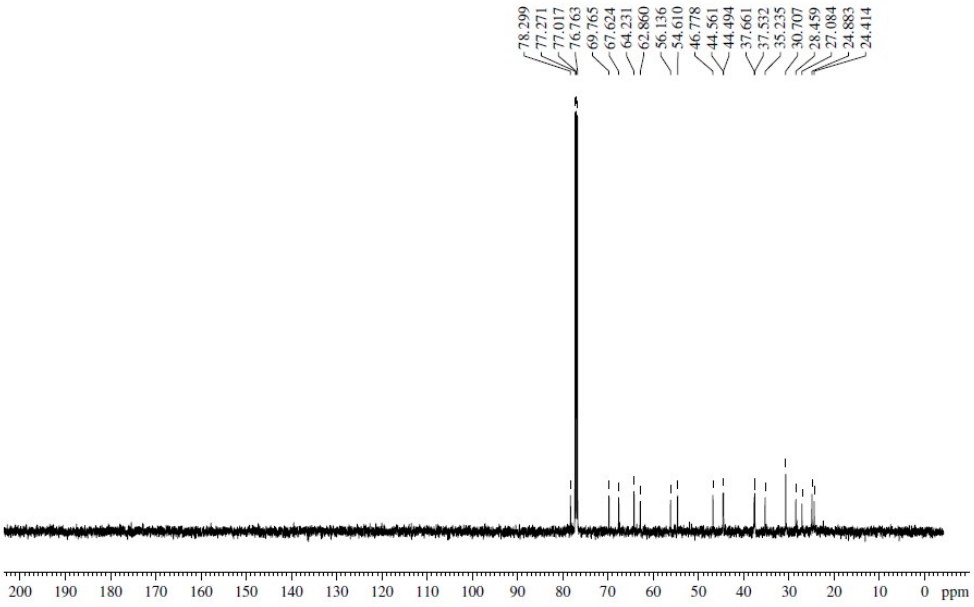
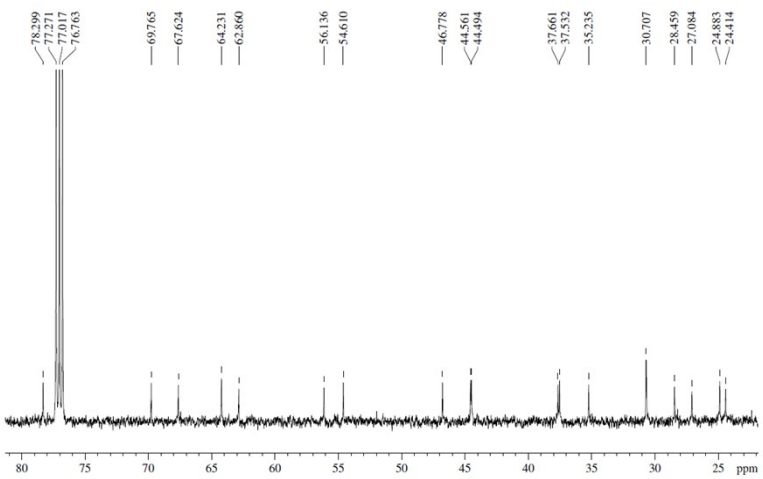
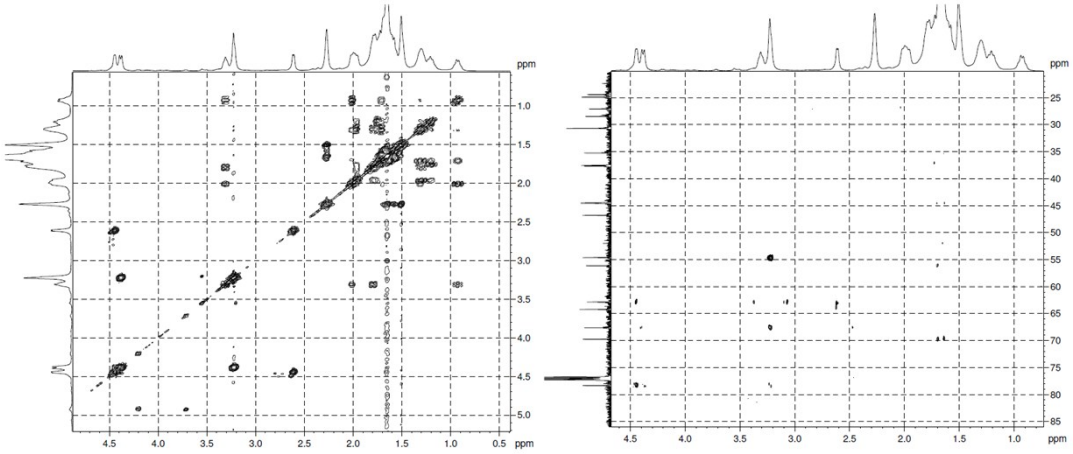


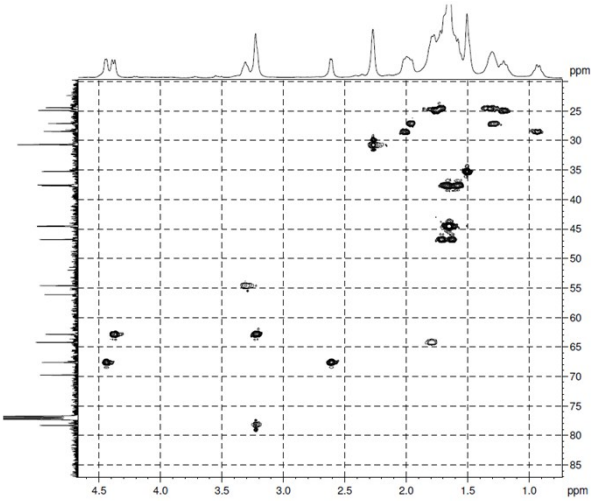
Figure 13. NMR and MS spectra of compound **14**.

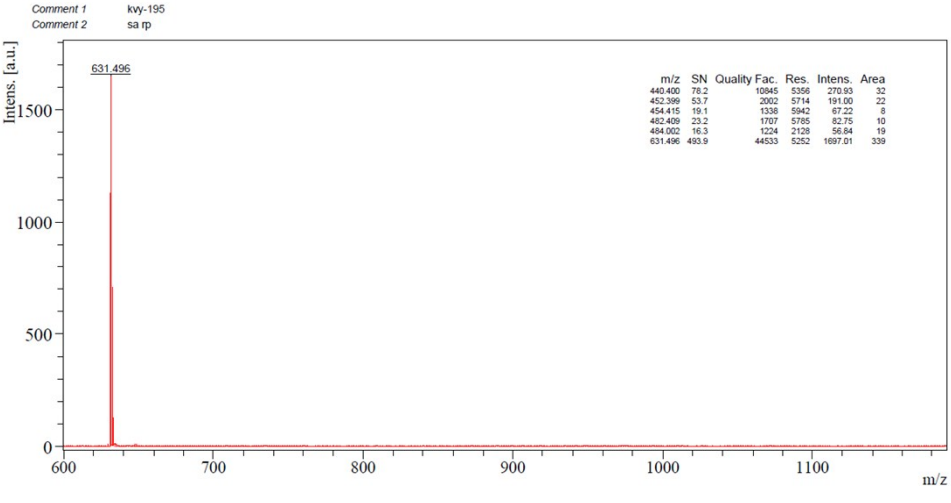





78.299
77.271
77.017
76.763
69.765
67.624
64.231
62.860
56.136
54.610
46.778
44.561
44.494
37.661
37.532
35.235
30.707
28.459
27.084
24.883
24.414
ppm


ppm


ppm


Comment 1 kvy-195
Comment 2 sa rp
631.496
Intens. [a.u.]
m/z SN Quality Fac. Res. Intens. Area
440.400 78.2 10845 5356 270.93 32
452.399 53.7 2002 5714 191.00 22
454.415 19.1 1338 5942 67.22 8
482.409 23.2 1707 5785 82.75 10
484.002 16.3 1224 2128 56.84 19
631.496 493.9 44533 5252 1697.01 339
m/z

Dimethyl *N′,N″*-(3b*R**,7a*R**,10b*R**,14a*R**)-tetradecahydro-1*H*,8*H*-2,3a,7b,9,10a,14b-hexaazadibenzo[*fg*,*op*]tetracene-2,9-diylbis(13′-isopropyl-4′,10′-dimethyl-23′,24′-dioxohexadecahydro-8′,12′-ethenonaphtho[2,1-*e*]isoindole-4′-carboxylate) (**15**)

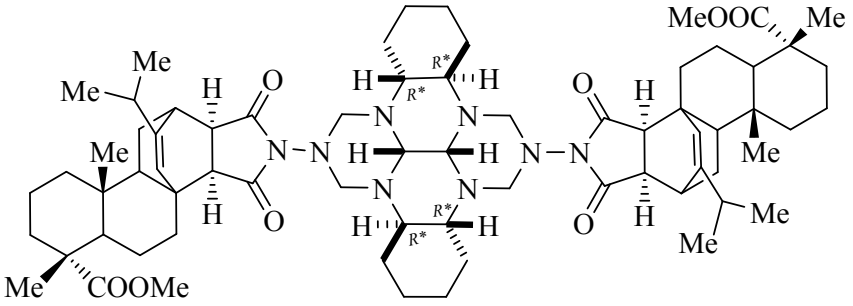
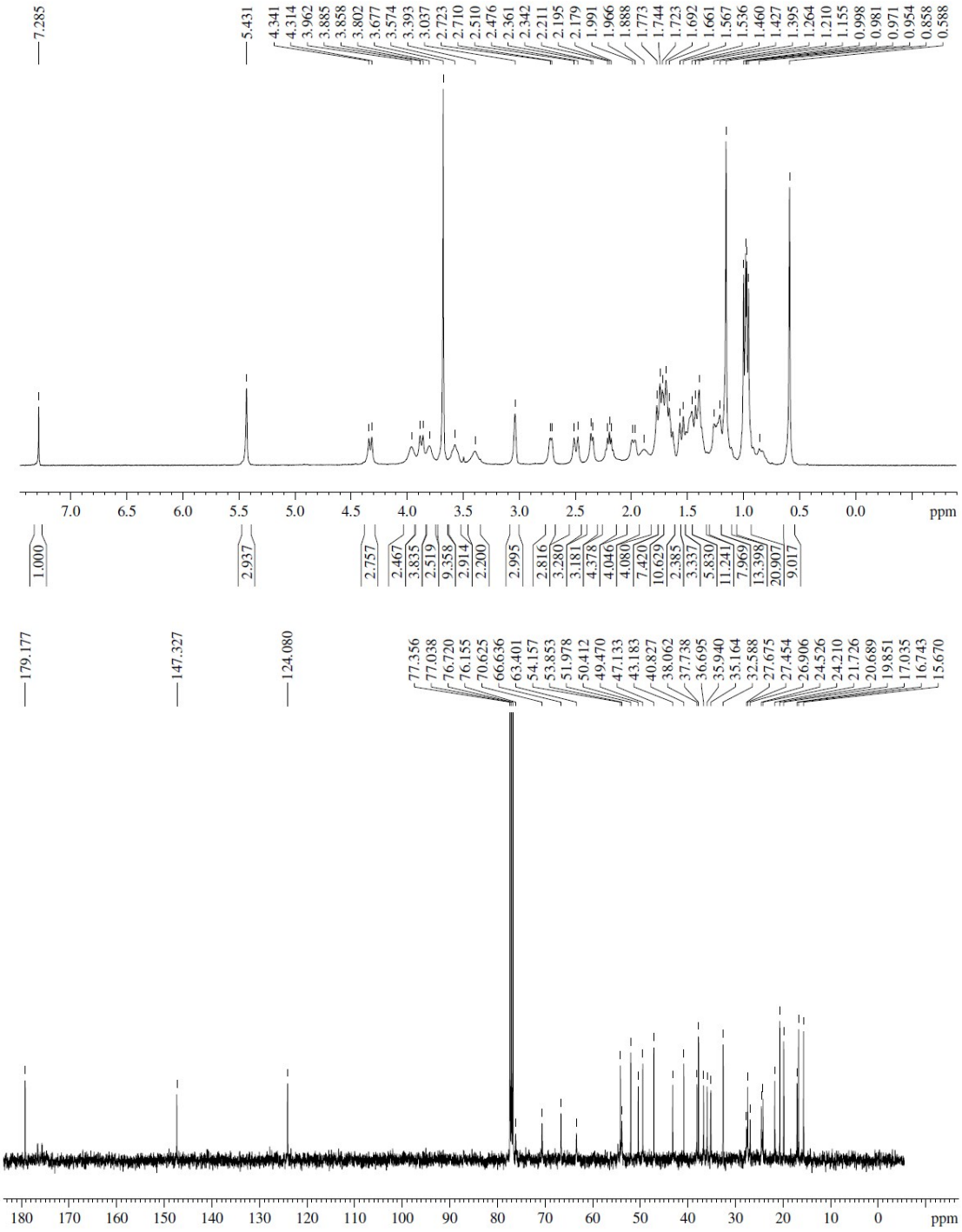
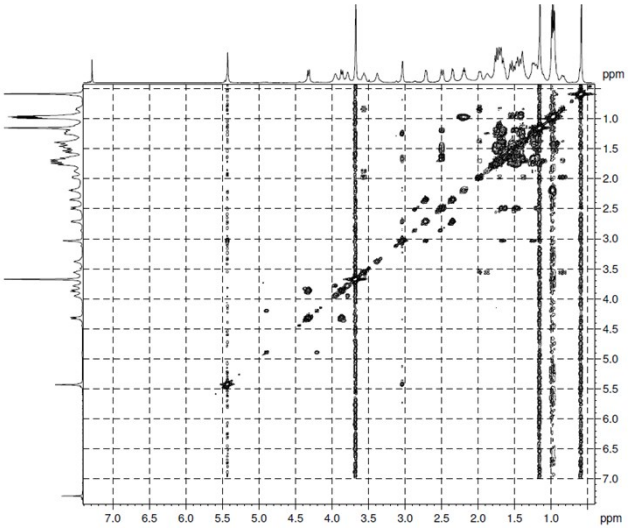
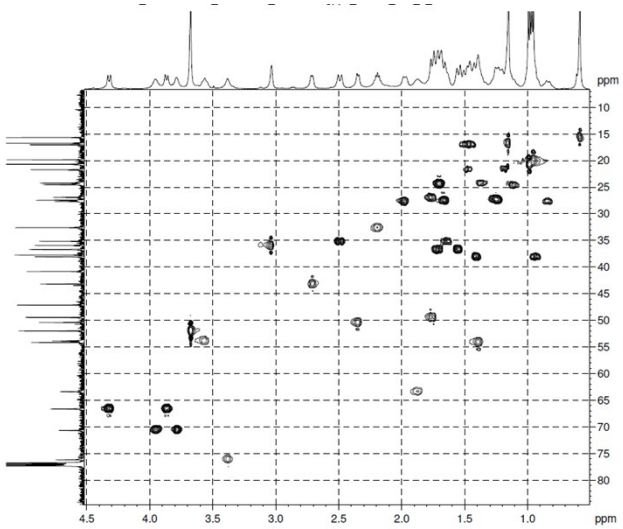
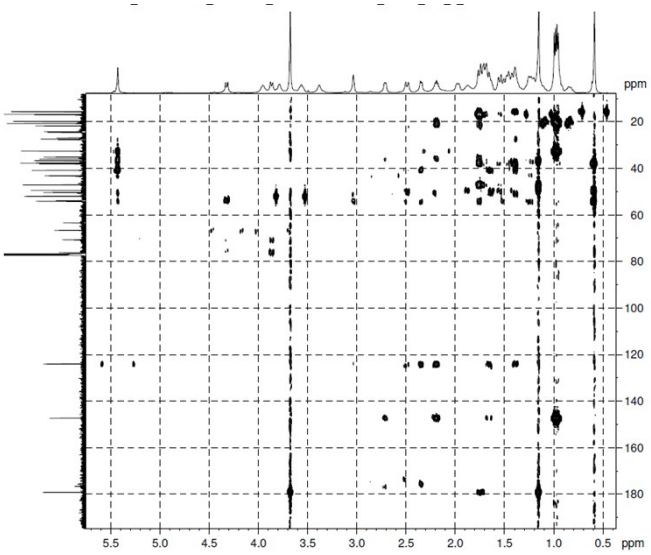


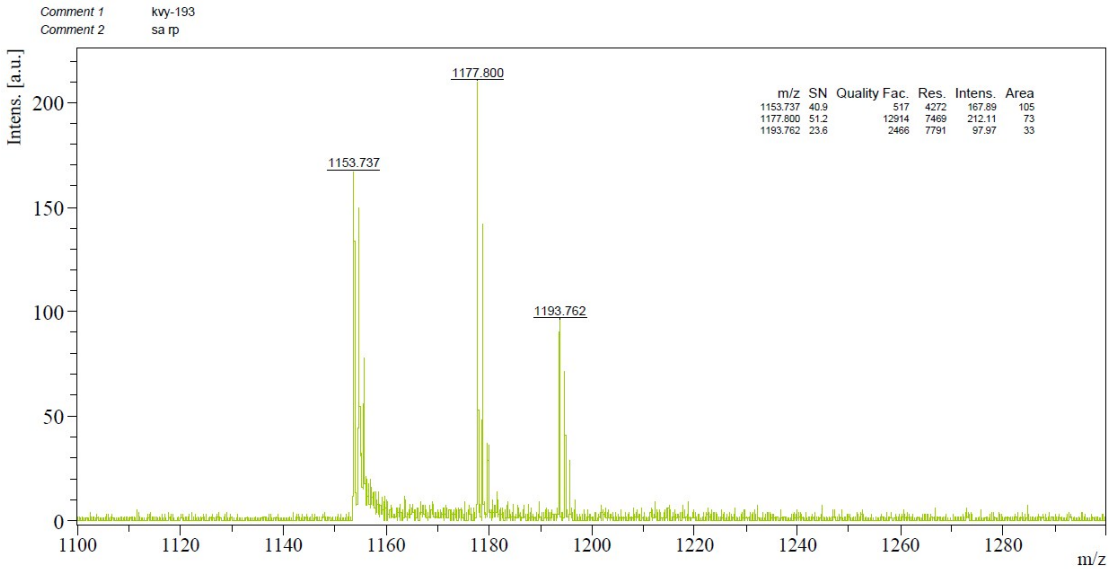
Figure 14. NMR and MS spectra of compound **15**.




ppm
7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm


ppm
4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm


ppm
5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm


Comment 1 kvy-193
Comment 2 sa rp
Intens. [a.u.]
1177.800
1153.737
1193.762
m/z SN Quality Fac. Res. Intens. Area
1153.737 40.9 517 4272 167.89 105
1177.800 51.2 12914 7469 212.11 73
1193.762 23.6 2466 7791 97.97 33
m/z

Dimethyl *N′,N″*-[(3b*R**,7a*R**,10b*R**,14a*R**)-tetradecahydro-1*H*,8*H*-2,3a,7b,9,10a,14b-hexaazadibenzo[*fg*,*op*]tetracene-2,9-diylbis(ethane-*N′,N″*-diyl)]bis(13′-isopropyl-4′,10′-dimethyl-23′,24′-dioxohexadecahydro-8′,12′-ethenonaphtho[2,1-*e*]isoindole-4′-carboxylate) (**16**)

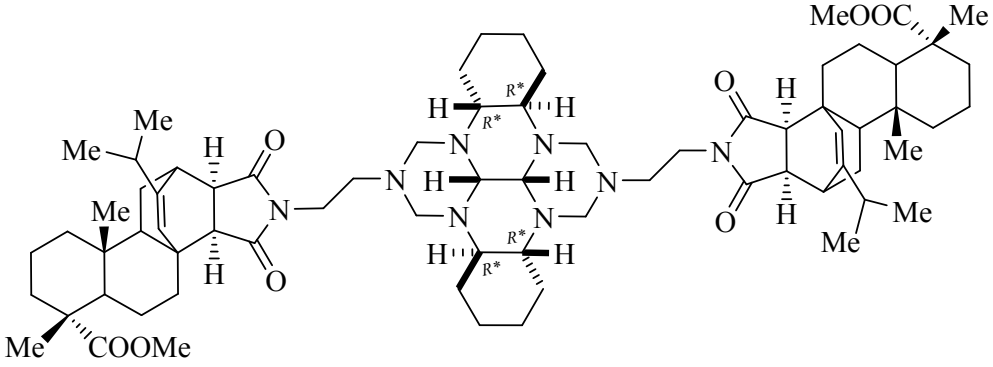
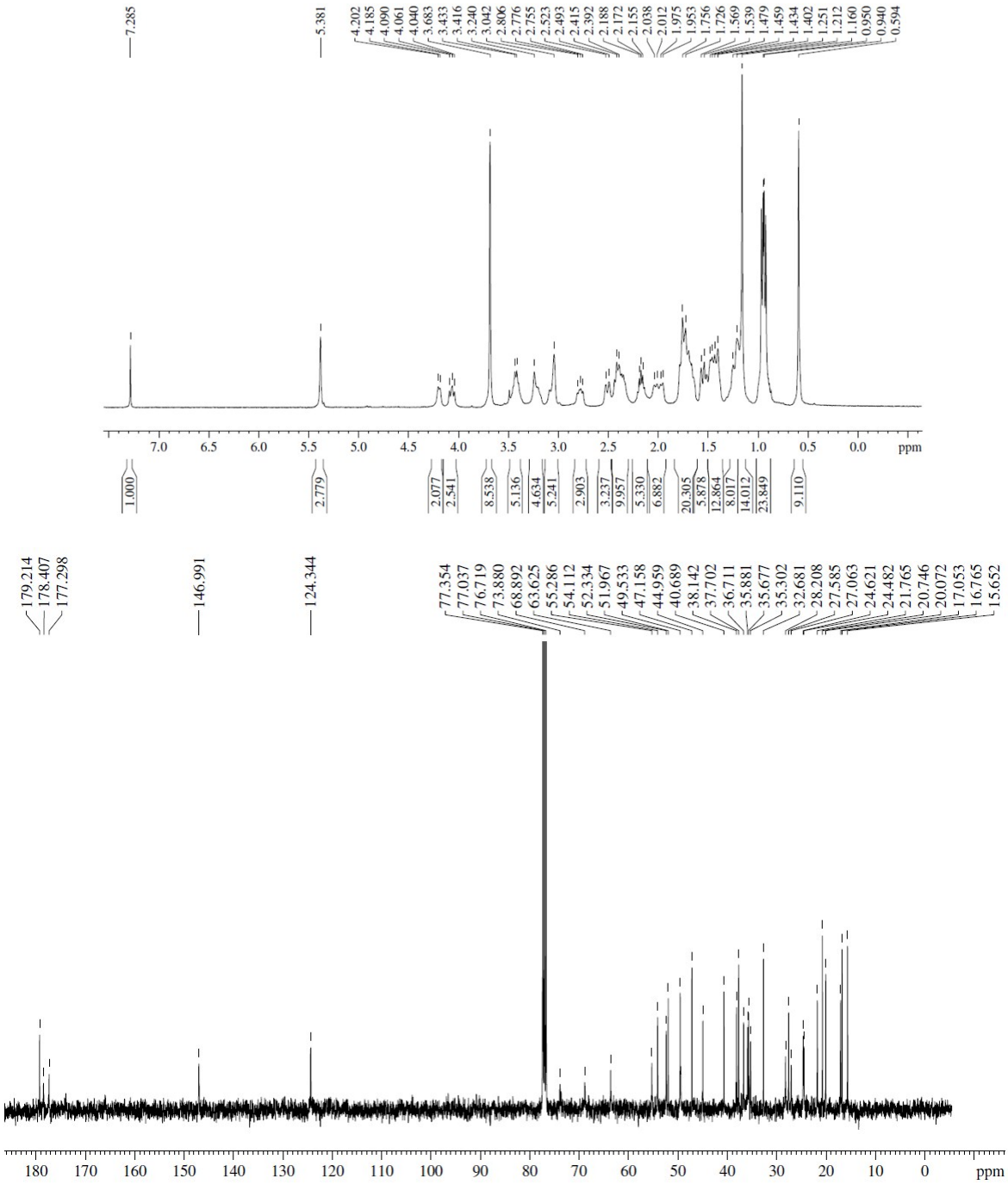
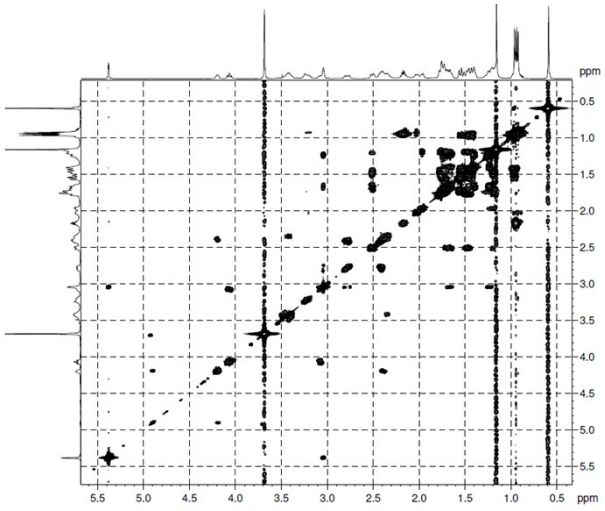
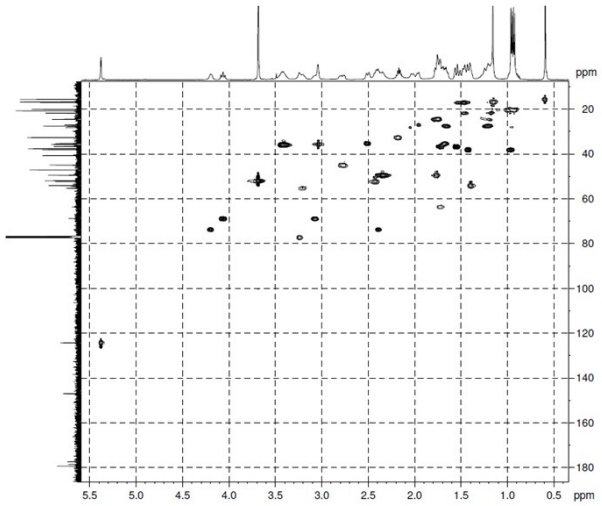
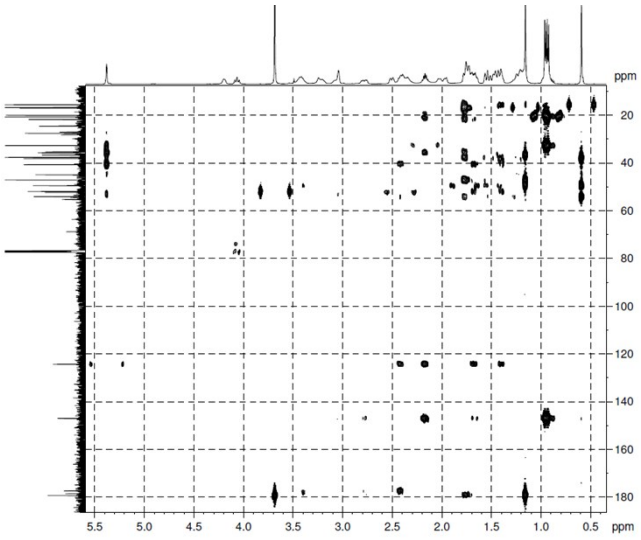


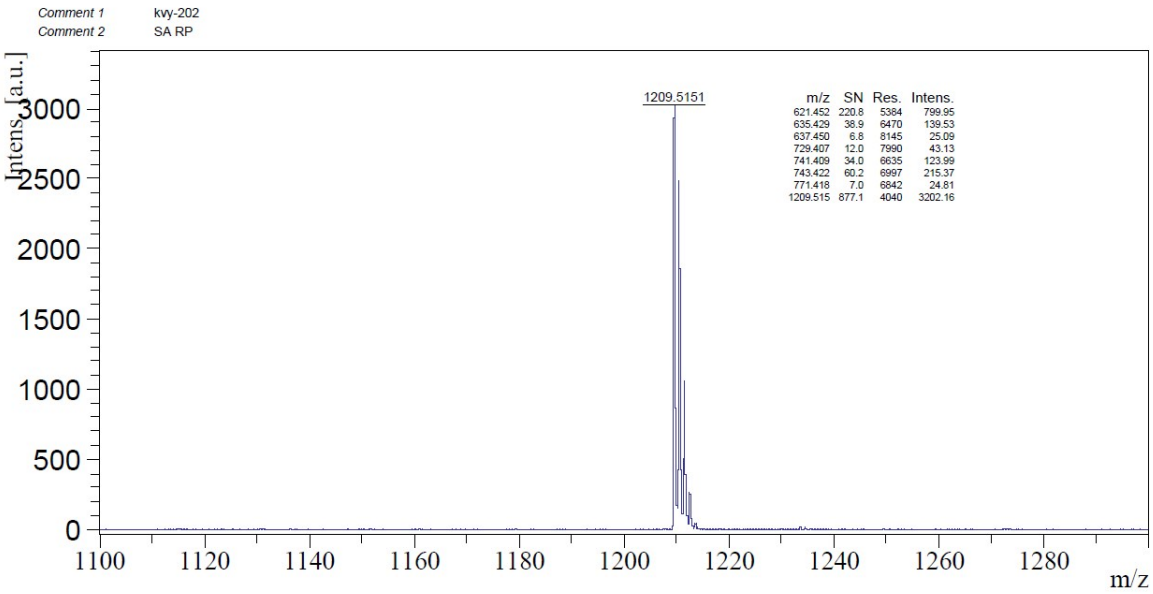
Figure 15. NMR and MS spectra of compound **16**.




ppm
5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm


ppm
5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm


ppm
5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm


Comment 1 kvy-202
Comment 2 SA RP
Intens. [a.u.]
1209.5151
m/z SN Res. Intens.
621.452 220.8 5384 799.95
635.429 38.9 6470 139.53
637.450 6.8 8145 25.09
729.407 12.0 7990 43.13
741.409 34.0 6635 123.99
743.422 60.2 6997 215.37
771.418 7.0 6842 24.81
1209.515 877.1 4040 3202.16
m/z

X-ray data of compound **9**

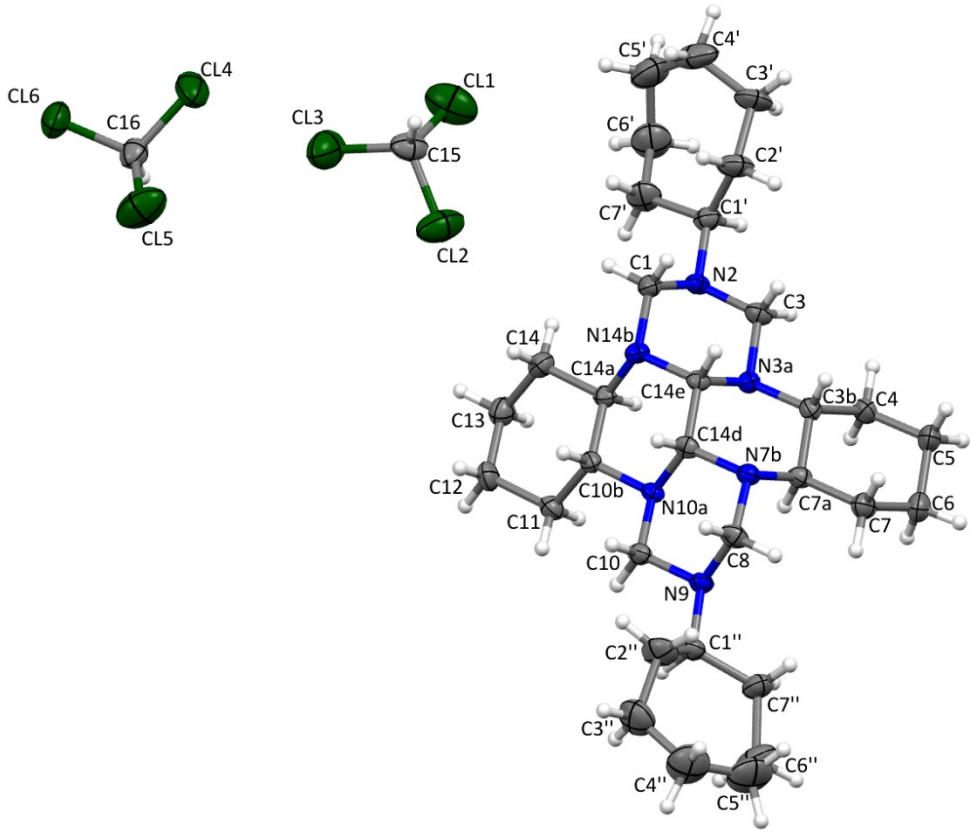


Figure 16. The independent part of the unit cell of compound **9**. Non-hydrogen atoms are represented by thermal vibration ellipsoids (p = 30%)

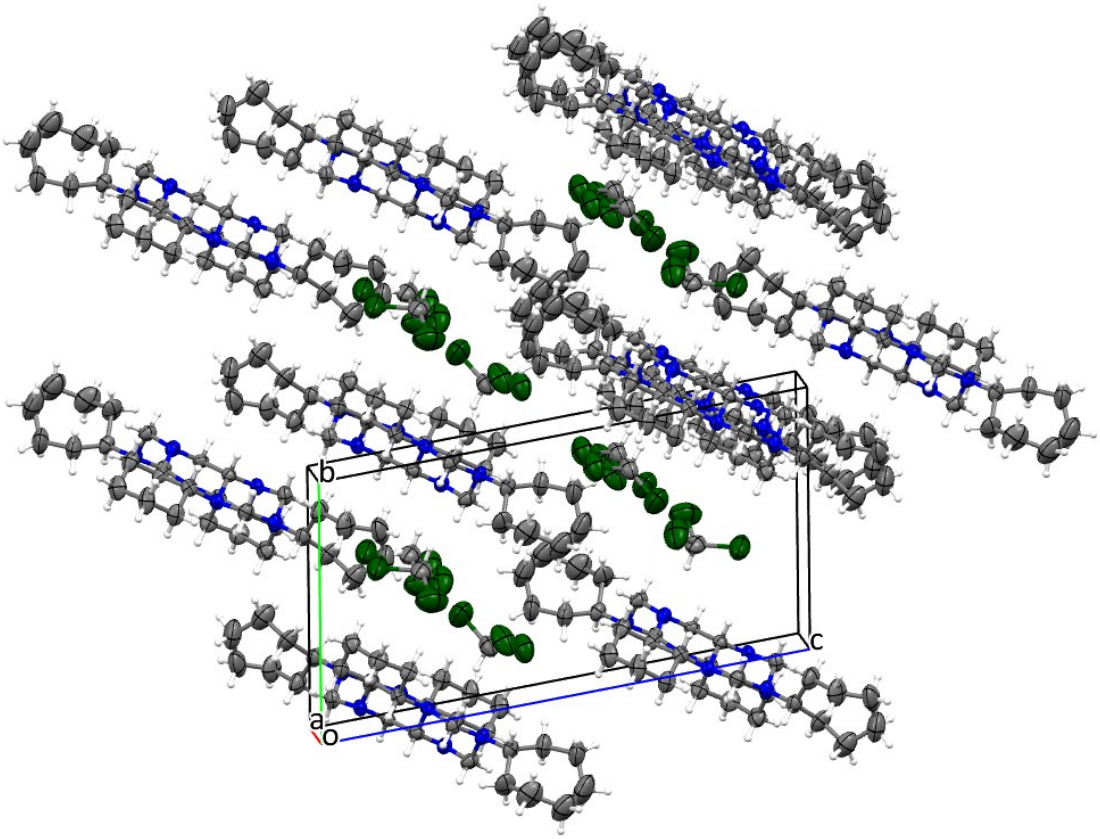


Figure 17. Packing of molecules in **9**,view along *a* axis.

Table 1. Crystal data and structure refinement for compound 9.

CCDC	1973770
Empirical formula	$C_{34}H_{58}Cl_6N_6$
Formula weight	763.56
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	10.1228(10)
b/Å	10.5481(11)
c/Å	19.5768(19)
α/°	78.370(9)
β/°	85.218(8)
γ/°	72.376(9)
Volume/Å^3	1950.8(4)
Z	2
ρ_{calc}g/cm^3	1.300
μ/mm^{-1}	0.473
F(000)	812.0
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.224 to 58.498
Index ranges	-12 ≤ h ≤ 12, -12 ≤ k ≤ 13, -24 ≤ l ≤ 23
Reflections collected	16427
Independent reflections	8968 [R_{int} = 0.0824]
Goodness-of-fit on F^2	0.872
Final R indexes [I>=2σ (I)]	R_1 = 0.0751, wR_2 = 0.1721
Final R indexes [all data]	R_1 = 0.2600, wR_2 = 0.2723
Largest diff. peak/hole / e Å^{-3}	0.32/-0.30

Table 2. Bond Lengths for compound **9**, Å.

Bond		Bond	
Cl(6)–C(16)	1.727(5)	C(10B)–C(11)	1.528(6)
Cl(4)–C(16)	1.757(5)	C(14A)–C(14)	1.532(6)
Cl(5)–C(16)	1.709(6)	C(3B)–C(7A)	1.505(6)
Cl(2)–C(15)	1.737(6)	C(3B)–C(4)	1.538(6)
N(10A)–C(10)	1.468(5)	C(1")–C(7")	1.531(7)
N(10A)–C(14D)	1.475(5)	C(1")–C(2")	1.531(7)
N(10A)–C(10B)	1.478(5)	C(7A)–C(7)	1.524(6)
N(9)–C(10)	1.449(5)	C(7)–C(6)	1.532(7)
N(9)–C(8)	1.464(5)	C(1')–C(7')	1.527(7)
N(9)–C(1")	1.471(5)	C(1')–C(2')	1.530(7)
Cl(3)–C(15)	1.733(6)	C(11)–C(12)	1.513(6)
N(3A)–C(14E)	1.473(5)	C(14)–C(13)	1.528(6)
N(3A)–C(3B)	1.469(5)	C(7')–C(6')	1.501(7)
N(3A)–C(3)	1.472(5)	C(13)–C(12)	1.514(6)
Cl(1)–C(15)	1.731(6)	C(7")–C(6")	1.529(8)
N(14B)–C(14E)	1.441(5)	C(6)–C(5)	1.514(7)
N(14B)–C(14A)	1.481(5)	C(4)–C(5)	1.524(6)
N(14B)–C(1)	1.437(5)	C(2')–C(3')	1.519(7)

N(7B)–C(14D)	1.454(5)	C(6")–C(5")	1.471(10)
N(7B)–C(8)	1.445(5)	C(2")–C(3")	1.483(8)
N(7B)–C(7A)	1.487(6)	C(3")–C(4")	1.508(9)
N(2)–C(3)	1.448(6)	C(3')–C(4')	1.481(8)
N(2)–C(1)	1.457(6)	C(4")–C(5")	1.452(10)
N(2)–C(1')	1.469(5)	C(6')–C(5')	1.502(10)
C(14E)–C(14D)	1.498(6)	C(5')–C(4')	1.488(9)
C(10B)–C(14A)	1.517(6)		

Table 3.Bond Angles for compound **9**, °

Angle		Angle	
Cl(6)–C(16)–Cl(4)	109.4(3)	C(7A)–C(3B)–C(4)	109.5(4)
Cl(5)–C(16)–Cl(6)	112.1(3)	N(7B)–C(8)–N(9)	111.5(3)
Cl(5)–C(16)–Cl(4)	110.3(3)	N(2)–C(3)–N(3A)	112.0(3)
C(10)–N(10A)–C(14D)	107.4(3)	N(9)–C(1")–C(7")	108.2(4)
C(10)–N(10A)–C(10B)	111.2(3)	N(9)–C(1")–C(2")	115.9(4)
C(14D)–N(10A)–C(10B)	109.6(3)	C(2")–C(1")–C(7")	114.9(5)
C(10)–N(9)–C(8)	108.6(4)	N(7B)–C(7A)–C(3B)	109.3(4)
C(10)–N(9)–C(1")	112.4(3)	N(7B)–C(7A)–C(7)	110.7(4)
C(8)–N(9)–C(1")	114.1(3)	C(3B)–C(7A)–C(7)	111.6(4)
C(3B)–N(3A)–C(14E)	109.1(3)	N(14B)–C(1)–N(2)	111.0(4)
C(3B)–N(3A)–C(3)	110.8(3)	C(7A)–C(7)–C(6)	111.9(4)
C(3)–N(3A)–C(14E)	107.9(4)	N(2)–C(1')–C(7')	109.7(4)
C(14E)–N(14B)–C(14A)	111.3(3)	N(2)–C(1')–C(2')	115.4(4)
C(1)–N(14B)–C(14E)	108.1(3)	C(7')–C(1')–C(2')	111.6(5)
C(1)–N(14B)–C(14A)	116.8(4)	C(12)–C(11)–C(10B)	111.6(4)
C(14D)–N(7B)–C(7A)	112.0(4)	C(13)–C(14)–C(14A)	112.2(4)
C(8)–N(7B)–C(14D)	108.3(3)	C(6')–C(7')–C(1')	115.6(5)
C(8)–N(7B)–C(7A)	116.1(4)	C(12)–C(13)–C(14)	111.0(4)
C(3)–N(2)–C(1)	109.4(4)	C(6")–C(7")–C(1")	116.2(5)
C(3)–N(2)–C(1')	112.5(3)	C(11)–C(12)–C(13)	110.4(4)
C(1)–N(2)–C(1')	115.3(4)	C(5)–C(6)–C(7)	110.5(5)
N(3A)–C(14E)–C(14D)	112.7(4)	C(5)–C(4)–C(3B)	111.8(4)
N(14B)–C(14E)–N(3A)	111.9(4)	C(3')–C(2')–C(1')	117.1(5)
N(14B)–C(14E)–C(14D)	110.5(3)	C(6)–C(5)–C(4)	110.7(4)
N(9)–C(10)–N(10A)	110.1(3)	C(5")–C(6")–C(7")	116.0(7)
N(10A)–C(14D)–C(14E)	112.4(3)	C(3")–C(2")–C(1")	116.4(6)
N(7B)–C(14D)–N(10A)	112.1(4)	Cl(3)–C(15)–Cl(2)	110.1(3)
N(7B)–C(14D)–C(14E)	110.4(3)	Cl(1)–C(15)–Cl(2)	111.1(4)
N(10A)–C(10B)–C(14A)	110.3(3)	Cl(1)–C(15)–Cl(3)	110.2(3)
N(10A)–C(10B)–C(11)	112.2(4)	C(2")–C(3")–C(4")	116.9(6)
C(14A)–C(10B)–C(11)	111.1(4)	C(4')–C(3')–C(2')	114.2(5)
N(14B)–C(14A)–C(10B)	108.1(3)	C(5")–C(4")–C(3")	121.1(7)
N(14B)–C(14A)–C(14)	110.3(4)	C(7')–C(6')–C(5')	115.1(7)
C(10B)–C(14A)–C(14)	110.7(3)	C(4')–C(5')–C(6')	119.9(6)
N(3A)–C(3B)–C(7A)	111.2(3)	C(3')–C(4')–C(5')	118.6(6)
N(3A)–C(3B)–C(4)	111.0(4)	C(4")–C(5")–C(6")	120.9(7)