

Table 2. Crystal data and structure refinement for 6d.

Empirical formula	C18 H35 I N4 O
Formula weight	450.40
Temperature	198(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 9.39150(10) Å alpha = 112.0790(10) deg b = 11.3046(2) Å beta = 94.6220(10) deg c = 12.1343(3) Å gamma = 111.2810(10) deg V = 1076.69(3) Å ³ Z = 2
Density (calculated)	1.389 Mg/m ³
Absorption coefficient	1.499 mm ⁻¹
Crystal size	0.40 x 0.20 x 0.10 mm
Theta range for data collection	2.15 to 28.27 deg
Index ranges	-12 ≤ h ≤ 12, -14 ≤ k ≤ 10, -15 ≤ l ≤ 16
Collection method	0.3 deg ω scans for 0.1667 min/scan
Reflections collected	6460 [R(int) = 0.0402]
Independent reflections	4591 [3850 obs, I > 2sigma(I)]
Refinement (shift/err=0.003)	Full-matrix least-squares on F ²
Data / restraints / parameters	4591 / 0 / 221
Goodness-of-fit on F ²	1.116
Final R indices (obs data)	R1 = 0.0736, wR2 = 0.1740
R indices (all data)	R1 = 0.0897, wR2 = 0.1939
calc w=1/[\s^2^(Fo^2^)+(0.0690P)^2^+6.1110P] where P=(Fo^2^+2Fc^2^)/3	
Extinction coefficient	0.0004(14)
Largest diff. peak and hole	1.651 and -0.877 e.Å ⁻³

Table 3. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 6d. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor

	x	y	z	U(eq)
I(1)	1476(1)	2620(1)	8303(1)	59(1)
N(4)	2451(7)	9089(6)	9796(7)	51(2)
C(5)	2448(8)	6523(7)	10947(7)	45(2)
N(1)	3157(8)	7712(7)	10613(6)	65(2)
N(2)	3686(7)	7092(7)	8263(7)	54(2)
C(14)	1908(9)	7619(8)	9505(10)	69(3)
C(6)	4717(9)	8024(9)	10375(9)	63(2)
C(7)	4635(9)	6870(10)	9088(8)	64(2)
C(4)	3464(10)	6658(9)	12048(8)	63(2)
C(3)	2669(10)	5395(10)	12330(9)	72(2)
C(15)	2086(11)	6694(10)	8432(12)	85(3)
N(3)	1184(10)	6895(14)	7421(11)	129(5)
C(13)	3188(12)	9116(10)	11658(11)	84(3)
C(1)	2931(12)	4192(12)	13622(10)	82(3)
C(12)	2595(14)	9773(10)	11070(11)	87(3)
C(10)	1647(15)	8195(16)	7548(14)	132(7)
C(2)	3635(12)	5471(12)	13424(10)	79(3)
C(9)	1844(16)	6107(20)	6302(13)	119(5)
C(11)	1354(13)	9167(16)	8945(18)	134(7)
C(8)	3394(13)	6273(16)	6951(10)	108(5)
O(1)	4115(9)	11132(9)	14274(7)	101(3)
C(16)	2973(11)	10799(10)	14687(8)	68(2)
C(17)	2690(13)	9836(13)	15272(11)	86(3)
C(18)	1744(14)	11314(13)	14589(11)	90(3)

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 6d. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
I(1)	58(1)	42(1)	72(1)	22(1)	28(1)	18(1)
N(4)	40(3)	50(3)	74(4)	40(3)	18(3)	16(3)
C(5)	37(3)	40(3)	57(4)	27(3)	12(3)	10(3)
N(1)	53(4)	60(4)	56(4)	31(3)	6(3)	-9(3)
N(2)	37(3)	60(4)	72(4)	37(3)	25(3)	16(3)
C(14)	40(4)	42(4)	101(7)	19(4)	33(4)	4(3)
C(6)	43(4)	67(5)	74(6)	38(4)	11(4)	12(4)
C(7)	37(4)	70(5)	72(5)	35(4)	8(4)	8(3)
C(4)	51(4)	56(4)	70(5)	36(4)	5(4)	3(3)
C(3)	51(5)	75(6)	73(6)	40(5)	7(4)	4(4)
C(15)	55(5)	61(5)	146(10)	50(6)	55(6)	22(4)

N(3)	44(4)	197(12)	146(10)	147(10)	-21(5)	-13(6)
C(13)	69(6)	52(5)	96(8)	4(5)	25(5)	16(4)
C(1)	64(6)	99(7)	88(7)	59(6)	13(5)	21(5)
C(12)	100(8)	47(5)	99(8)	34(5)	43(6)	9(5)
C(10)	84(8)	145(12)	135(12)	120(11)	-32(8)	-33(8)
C(2)	59(5)	85(7)	85(7)	45(6)	11(5)	16(5)
C(9)	84(8)	192(16)	94(9)	80(10)	41(7)	47(9)
C(11)	60(6)	151(12)	272(21)	183(15)	37(9)	36(7)
C(8)	63(6)	159(12)	73(7)	68(8)	0(5)	3(7)
O(1)	71(5)	113(6)	81(5)	33(5)	28(4)	8(4)
C(16)	57(5)	74(6)	44(4)	15(4)	4(4)	10(4)
C(17)	69(6)	107(8)	104(8)	61(7)	37(6)	44(6)
C(18)	87(7)	96(8)	92(8)	61(7)	13(6)	25(6)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 6d.

	x	y	z	U(eq)
H(5A)	2248(8)	5630(7)	10237(7)	54
H(5B)	1417(8)	6470(7)	11114(7)	54
H(14)	802(9)	7224(8)	9585(10)	83
H(6A)	5434(9)	8049(9)	11037(9)	75
H(6B)	5154(9)	8965(9)	10378(9)	75
H(7A)	5697(9)	7044(10)	8937(8)	76
H(7B)	4119(9)	5905(10)	9027(8)	76
H(4A)	3654(10)	7540(9)	12768(8)	76
H(4B)	4499(10)	6711(9)	11890(8)	76
H(3A)	1633(10)	5346(10)	12481(9)	86
H(3B)	2474(10)	4518(10)	11603(9)	86
H(15)	1597(11)	5699(10)	8325(12)	102
H(13A)	2527(12)	8873(10)	12205(11)	101
H(13B)	4282(12)	9762(10)	12162(11)	101
H(1A)	3633(48)	4273(40)	14315(49)	123
H(1B)	2786(90)	3364(15)	12880(29)	123
H(1C)	1905(46)	4091(48)	13801(75)	123
H(12A)	1552(14)	9699(10)	11220(11)	104
H(12B)	3323(14)	10785(10)	11402(11)	104
H(10A)	1023(15)	8213(16)	6861(14)	158
H(10B)	2776(15)	8598(16)	7551(14)	158
H(2A)	4705(12)	5609(12)	13308(10)	95
H(2B)	3745(12)	6300(12)	14167(10)	95
H(9A)	1107(16)	5099(20)	5827(13)	143
H(9B)	2006(16)	6565(20)	5740(13)	143
H(11A)	1627(13)	10153(16)	9084(18)	160
H(11B)	252(13)	8727(16)	8995(18)	160
H(8A)	3356(13)	5333(16)	6782(10)	130
H(8B)	4261(13)	6756(16)	6644(10)	130
H(17A)	1652(45)	9038(47)	14850(50)	128
H(17B)	2722(99)	10340(26)	16137(22)	128
H(17C)	3509(60)	9486(72)	15219(71)	128
H(18A)	785(38)	10537(27)	13979(60)	135

H(18B)	2130(43)	12075(66)	14333(81)	135
H(18C)	1506(77)	11669(87)	15389(22)	135

Table 6. Bond lengths [Å] and angles [deg] for 1.

N(4)-C(12)	1.414(13)
N(4)-C(14)	1.436(10)
N(4)-C(11)	1.449(13)
C(5)-N(1)	1.489(9)
C(5)-C(4)	1.502(11)
C(5)-H(5A)	0.99
C(5)-H(5B)	0.99
N(1)-C(6)	1.457(11)
N(1)-C(13)	1.604(12)
N(1)-C(14)	1.656(13)
N(2)-C(7)	1.438(11)
N(2)-C(8)	1.450(14)
N(2)-C(15)	1.460(10)
C(14)-C(15)	1.398(14)
C(14)-H(14)	1.00
C(6)-C(7)	1.588(13)
C(6)-H(6A)	0.99
C(6)-H(6B)	0.99
C(7)-H(7A)	0.99
C(7)-H(7B)	0.99
C(4)-C(3)	1.533(11)
C(4)-H(4A)	0.99
C(4)-H(4B)	0.99
C(3)-C(2)	1.502(13)
C(3)-H(3A)	0.99
C(3)-H(3B)	0.99
C(15)-N(3)	1.57(2)
C(15)-H(15)	1.00
N(3)-C(10)	1.31(2)
N(3)-C(9)	1.63(2)
C(13)-C(12)	1.42(2)
C(13)-H(13A)	0.99
C(13)-H(13B)	0.99
C(1)-C(2)	1.475(14)
C(1)-H(1A)	0.98
C(1)-H(1B)	0.98
C(1)-H(1C)	0.9800(12)
C(12)-H(12A)	0.99
C(12)-H(12B)	0.99
C(10)-C(11)	1.75(2)
C(10)-H(10A)	0.99
C(10)-H(10B)	0.99
C(2)-H(2A)	0.99
C(2)-H(2B)	0.99
C(9)-C(8)	1.51(2)
C(9)-H(9A)	0.99
C(9)-H(9B)	0.99
C(11)-H(11A)	0.99
C(11)-H(11B)	0.99

C(8)-H(8A)	0.99
C(8)-H(8B)	0.99
O(1)-C(16)	1.216(11)
C(16)-C(17)	1.471(14)
C(16)-C(18)	1.48(2)
C(17)-H(17A)	0.98
C(17)-H(17B)	0.98
C(17)-H(17C)	0.9800(12)
C(18)-H(18A)	0.98
C(18)-H(18B)	0.980(2)
C(18)-H(18C)	0.98
C(12)-N(4)-C(14)	105.4(7)
C(12)-N(4)-C(11)	119.0(10)
C(14)-N(4)-C(11)	105.8(8)
N(1)-C(5)-C(4)	113.6(6)
N(1)-C(5)-H(5A)	108.8(4)
C(4)-C(5)-H(5A)	108.8(5)
N(1)-C(5)-H(5B)	108.8(4)
C(4)-C(5)-H(5B)	108.8(5)
H(5A)-C(5)-H(5B)	107.7
C(6)-N(1)-C(5)	118.3(7)
C(6)-N(1)-C(13)	108.9(6)
C(5)-N(1)-C(13)	108.9(7)
C(6)-N(1)-C(14)	111.0(6)
C(5)-N(1)-C(14)	111.8(5)
C(13)-N(1)-C(14)	95.5(7)
C(7)-N(2)-C(8)	118.6(8)
C(7)-N(2)-C(15)	109.9(7)
C(8)-N(2)-C(15)	101.8(8)
C(15)-C(14)-N(4)	120.4(8)
C(15)-C(14)-N(1)	103.5(8)
N(4)-C(14)-N(1)	100.2(6)
C(15)-C(14)-H(14)	110.6(5)
N(4)-C(14)-H(14)	110.6(4)
N(1)-C(14)-H(14)	110.6(4)
N(1)-C(6)-C(7)	111.0(7)
N(1)-C(6)-H(6A)	109.4(5)
C(7)-C(6)-H(6A)	109.4(5)
N(1)-C(6)-H(6B)	109.4(5)
C(7)-C(6)-H(6B)	109.4(4)
H(6A)-C(6)-H(6B)	108.0
N(2)-C(7)-C(6)	100.8(7)
N(2)-C(7)-H(7A)	111.6(4)
C(6)-C(7)-H(7A)	111.6(4)
N(2)-C(7)-H(7B)	111.6(4)
C(6)-C(7)-H(7B)	111.6(4)
H(7A)-C(7)-H(7B)	109.4
C(5)-C(4)-C(3)	110.7(6)
C(5)-C(4)-H(4A)	109.5(5)
C(3)-C(4)-H(4A)	109.5(6)
C(5)-C(4)-H(4B)	109.5(5)
C(3)-C(4)-H(4B)	109.5(5)
H(4A)-C(4)-H(4B)	108.1
C(2)-C(3)-C(4)	113.1(7)
C(2)-C(3)-H(3A)	109.0(6)
C(4)-C(3)-H(3A)	109.0(5)
C(2)-C(3)-H(3B)	109.0(6)

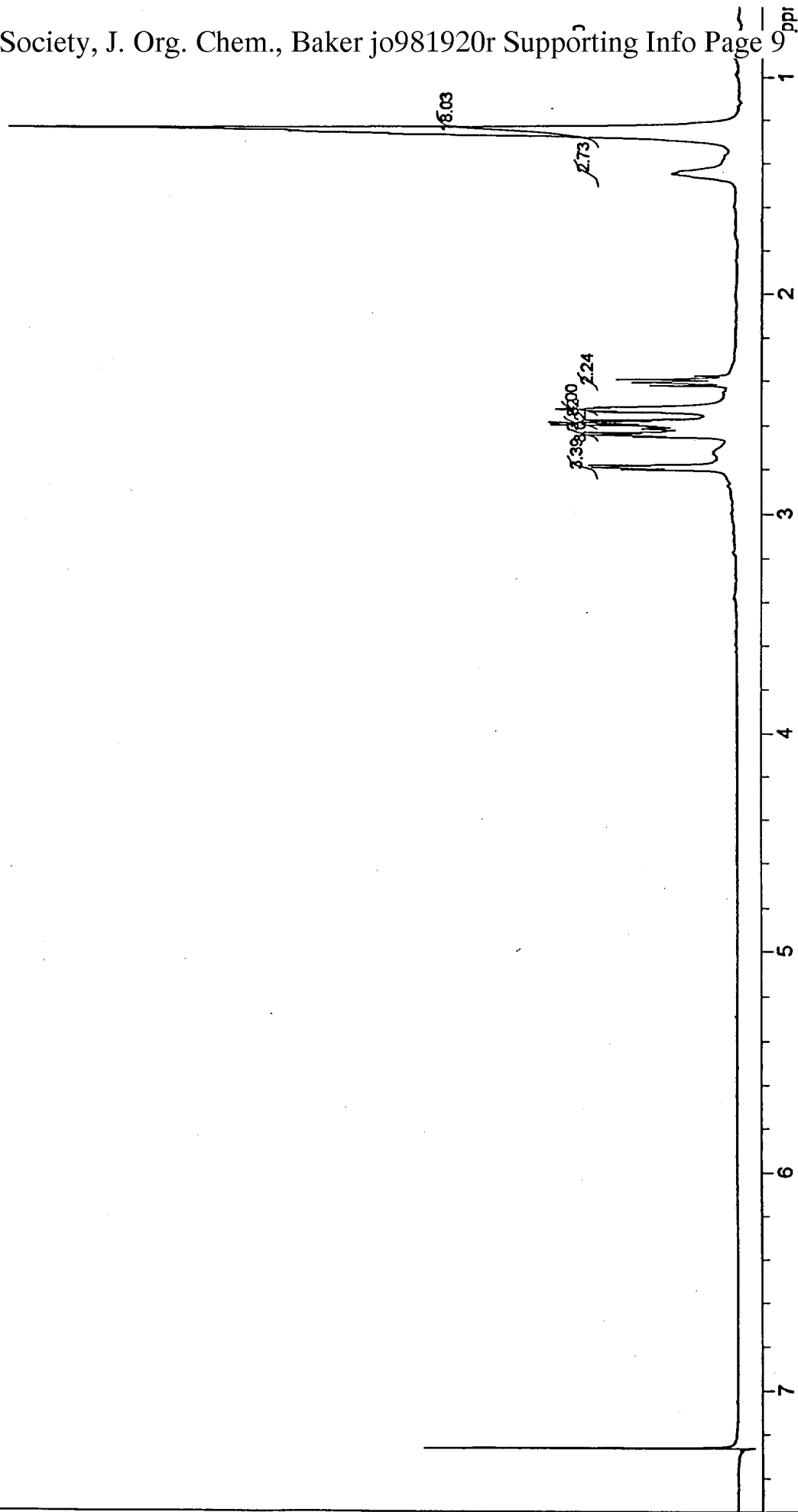
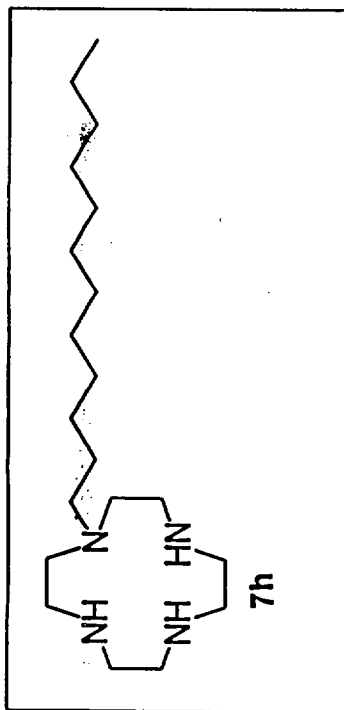
C(4)-C(3)-H(3B)	109.0(6)
H(3A)-C(3)-H(3B)	107.8
C(14)-C(15)-N(2)	115.9(9)
C(14)-C(15)-N(3)	101.6(10)
N(2)-C(15)-N(3)	103.8(8)
C(14)-C(15)-H(15)	111.6(5)
N(2)-C(15)-H(15)	111.6(5)
N(3)-C(15)-H(15)	111.6(5)
C(10)-N(3)-C(15)	116.2(9)
C(10)-N(3)-C(9)	106.2(12)
C(15)-N(3)-C(9)	96.5(10)
C(12)-C(13)-N(1)	107.9(9)
C(12)-C(13)-H(13A)	110.1(6)
N(1)-C(13)-H(13A)	110.1(5)
C(12)-C(13)-H(13B)	110.1(6)
N(1)-C(13)-H(13B)	110.1(5)
H(13A)-C(13)-H(13B)	108.4
C(2)-C(1)-H(1A)	109.5(6)
C(2)-C(1)-H(1B)	109.5(7)
H(1A)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1C)	109.5(6)
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.47(14)
N(4)-C(12)-C(13)	108.4(9)
N(4)-C(12)-H(12A)	110.0(6)
C(13)-C(12)-H(12A)	110.0(6)
N(4)-C(12)-H(12B)	110.0(4)
C(13)-C(12)-H(12B)	110.0(6)
H(12A)-C(12)-H(12B)	108.4
N(3)-C(10)-C(11)	107.1(11)
N(3)-C(10)-H(10A)	110.3(6)
C(11)-C(10)-H(10A)	110.3(6)
N(3)-C(10)-H(10B)	110.3(9)
C(11)-C(10)-H(10B)	110.3(6)
H(10A)-C(10)-H(10B)	108.6
C(1)-C(2)-C(3)	112.8(8)
C(1)-C(2)-H(2A)	109.0(6)
C(3)-C(2)-H(2A)	109.0(6)
C(1)-C(2)-H(2B)	109.0(7)
C(3)-C(2)-H(2B)	109.0(6)
H(2A)-C(2)-H(2B)	107.81(5)
C(8)-C(9)-N(3)	103.5(10)
C(8)-C(9)-H(9A)	111.1(9)
N(3)-C(9)-H(9A)	111.1(7)
C(8)-C(9)-H(9B)	111.1(7)
N(3)-C(9)-H(9B)	111.1(7)
H(9A)-C(9)-H(9B)	109.0
N(4)-C(11)-C(10)	100.5(10)
N(4)-C(11)-H(11A)	111.7(6)
C(10)-C(11)-H(11A)	111.7(5)
N(4)-C(11)-H(11B)	111.7(5)
C(10)-C(11)-H(11B)	111.7(5)
H(11A)-C(11)-H(11B)	109.4
N(2)-C(8)-C(9)	109.4(12)
N(2)-C(8)-H(8A)	109.8(7)
C(9)-C(8)-H(8A)	109.8(9)
N(2)-C(8)-H(8B)	109.8(5)

C(9)-C(8)-H(8B)	109.8(7)
H(8A)-C(8)-H(8B)	108.2
O(1)-C(16)-C(17)	122.8(10)
O(1)-C(16)-C(18)	121.3(10)
C(17)-C(16)-C(18)	115.9(9)
C(16)-C(17)-H(17A)	109.5(6)
C(16)-C(17)-H(17B)	109.5(6)
H(17A)-C(17)-H(17B)	109.5(2)
C(16)-C(17)-H(17C)	109.5(6)
H(17A)-C(17)-H(17C)	109.5(2)
H(17B)-C(17)-H(17C)	109.47(9)
C(16)-C(18)-H(18A)	109.5(6)
C(16)-C(18)-H(18B)	109.5(6)
H(18A)-C(18)-H(18B)	109.47(6)
C(16)-C(18)-H(18C)	109.5(6)
H(18A)-C(18)-H(18C)	109.5(2)
H(18B)-C(18)-H(18C)	109.47(13)

Table 7. Torsion angles [deg] for 1.

C(4)-C(5)-N(1)-C(6)	56.1(10)
C(4)-C(5)-N(1)-C(13)	-68.8(9)
C(4)-C(5)-N(1)-C(14)	-173.1(7)
C(12)-N(4)-C(14)-C(15)	-160.6(10)
C(11)-N(4)-C(14)-C(15)	72.5(12)
C(12)-N(4)-C(14)-N(1)	-48.2(8)
C(11)-N(4)-C(14)-N(1)	-175.1(9)
C(6)-N(1)-C(14)-C(15)	50.6(8)
C(5)-N(1)-C(14)-C(15)	-83.9(8)
C(13)-N(1)-C(14)-C(15)	163.3(7)
C(6)-N(1)-C(14)-N(4)	-74.3(8)
C(5)-N(1)-C(14)-N(4)	151.2(6)
C(13)-N(1)-C(14)-N(4)	38.3(7)
C(5)-N(1)-C(6)-C(7)	73.6(9)
C(13)-N(1)-C(6)-C(7)	-161.5(8)
C(14)-N(1)-C(6)-C(7)	-57.6(9)
C(8)-N(2)-C(7)-C(6)	176.7(7)
C(15)-N(2)-C(7)-C(6)	-66.9(8)
N(1)-C(6)-C(7)-N(2)	64.4(8)
N(1)-C(5)-C(4)-C(3)	-179.5(8)
C(5)-C(4)-C(3)-C(2)	179.9(9)
N(4)-C(14)-C(15)-N(2)	54.2(14)
N(1)-C(14)-C(15)-N(2)	-56.4(10)
N(4)-C(14)-C(15)-N(3)	-57.5(10)
N(1)-C(14)-C(15)-N(3)	-168.2(6)
C(7)-N(2)-C(15)-C(14)	73.3(11)
C(8)-N(2)-C(15)-C(14)	-160.1(11)
C(7)-N(2)-C(15)-N(3)	-176.3(9)
C(8)-N(2)-C(15)-N(3)	-49.7(11)
C(14)-C(15)-N(3)-C(10)	55(2)
N(2)-C(15)-N(3)-C(10)	-66(2)
C(14)-C(15)-N(3)-C(9)	166.6(8)
N(2)-C(15)-N(3)-C(9)	45.9(10)

C(6)-N(1)-C(13)-C(12)	96.8(9)
C(5)-N(1)-C(13)-C(12)	-132.9(8)
C(14)-N(1)-C(13)-C(12)	-17.6(9)
C(14)-N(4)-C(12)-C(13)	38.3(10)
C(11)-N(4)-C(12)-C(13)	156.8(8)
N(1)-C(13)-C(12)-N(4)	-9.8(11)
C(15)-N(3)-C(10)-C(11)	-61(2)
C(9)-N(3)-C(10)-C(11)	-166.8(9)
C(4)-C(3)-C(2)-C(1)	-174.8(10)
C(10)-N(3)-C(9)-C(8)	94.3(12)
C(15)-N(3)-C(9)-C(8)	-25.4(12)
C(12)-N(4)-C(11)-C(10)	179.5(7)
C(14)-N(4)-C(11)-C(10)	-62.3(8)
N(3)-C(10)-C(11)-N(4)	64.4(11)
C(7)-N(2)-C(8)-C(9)	152.5(10)
C(15)-N(2)-C(8)-C(9)	31.8(13)
N(3)-C(9)-C(8)-N(2)	-2.3(14)



STANDARD PROTON PARAMETERS

F1: 499,699

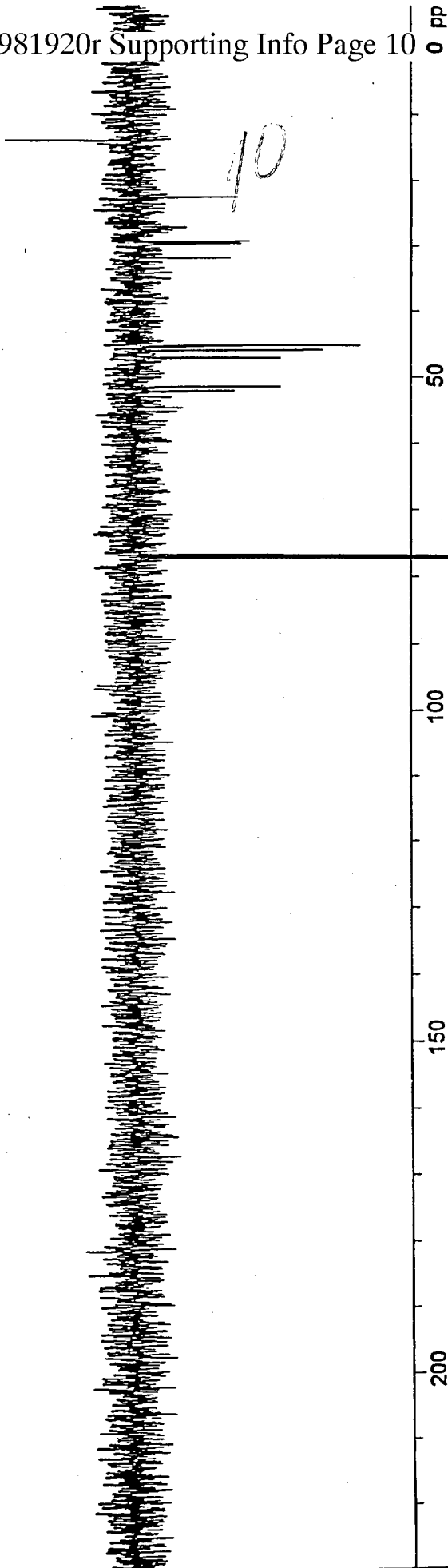
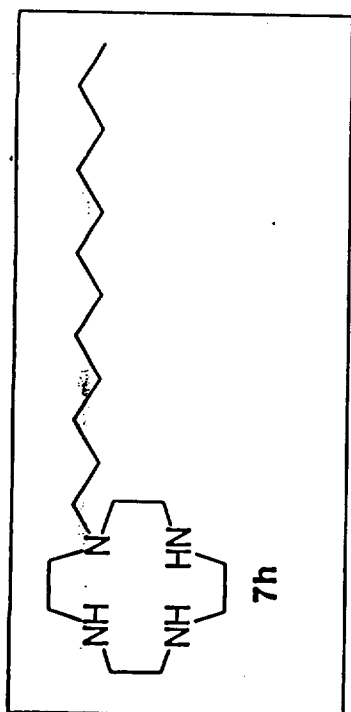
F2: 499,699

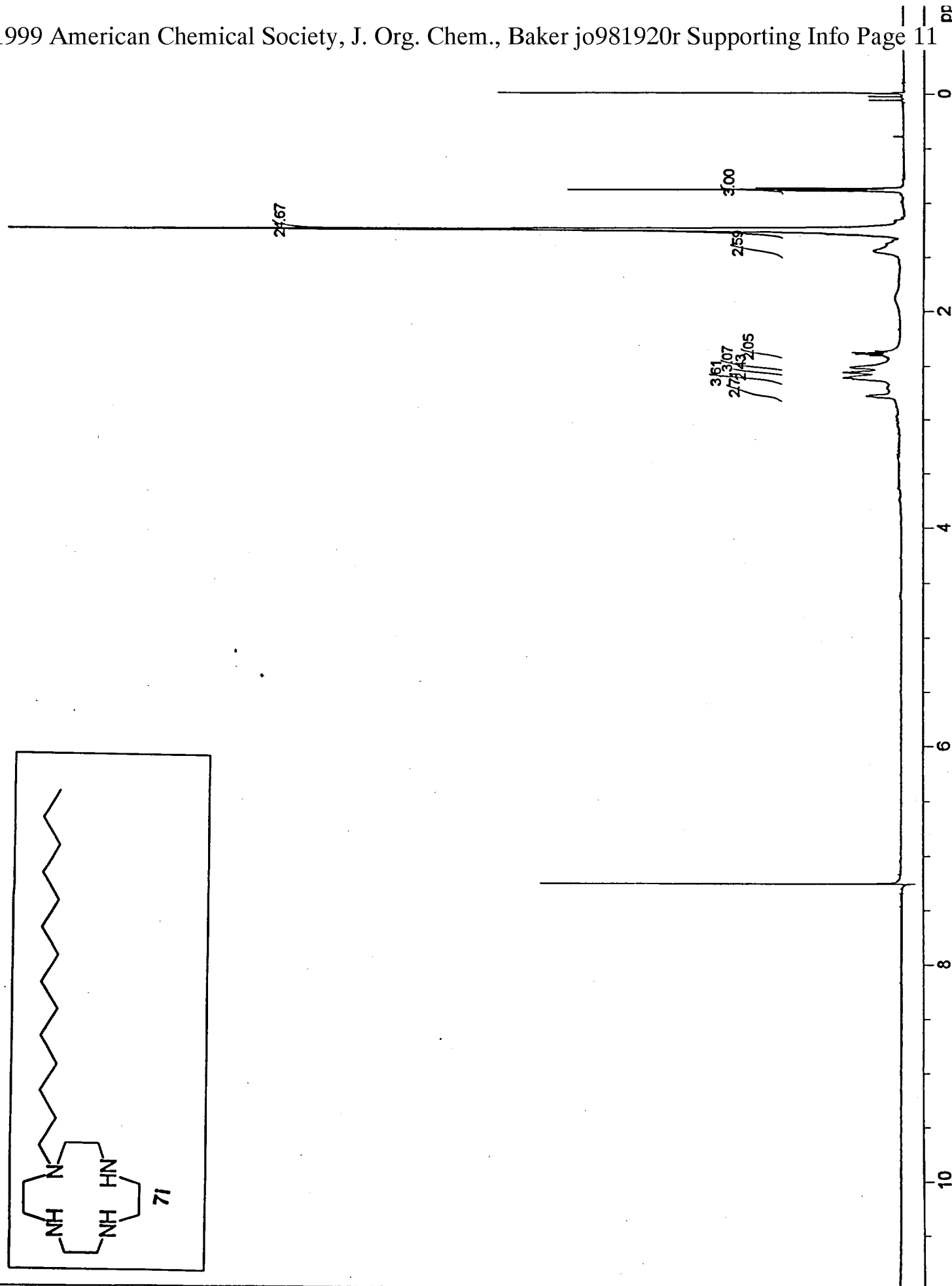
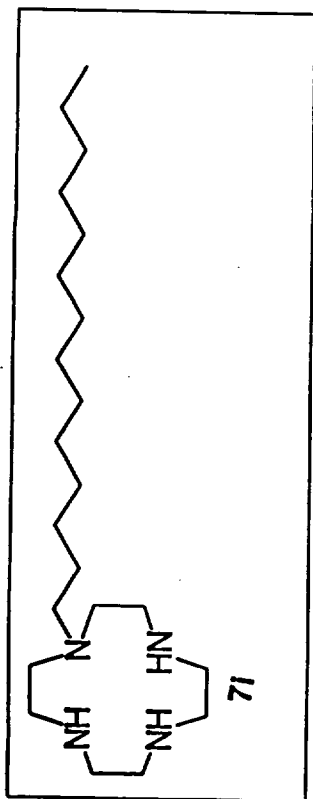
SW1: 5996

OF1: 2494.0

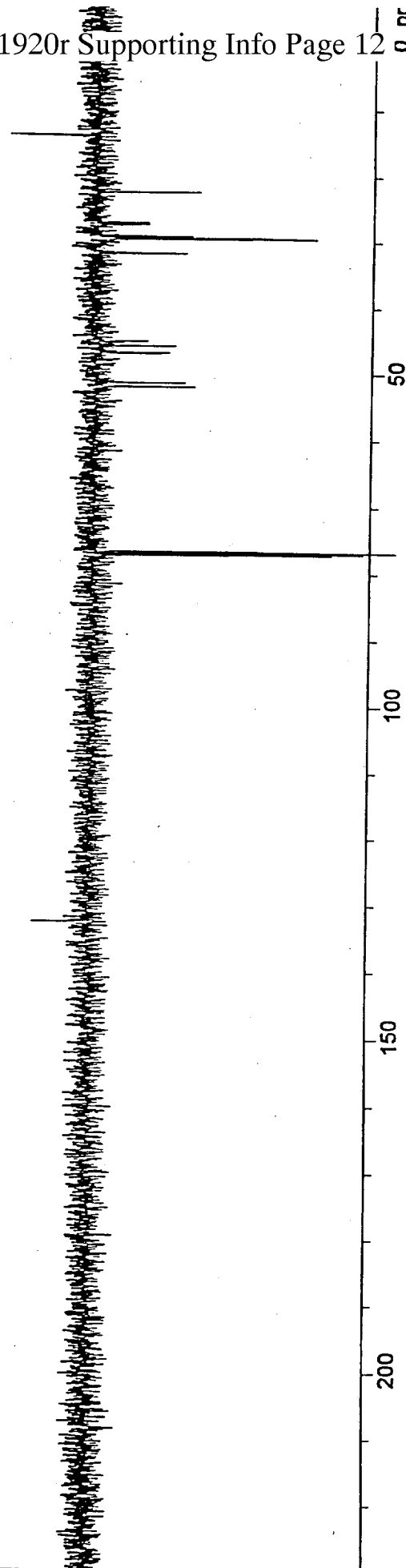
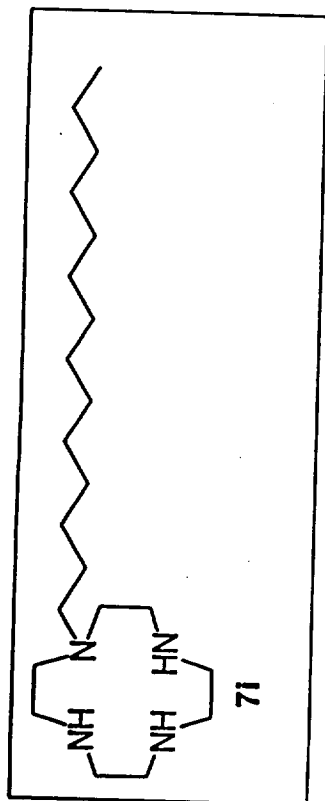
PTSId: 32768

USER: -- DATE: Sep 23 97





STANDARD PROTON PARAMETERS



STANDARD CARBON PARAMETERS

F1: 125.663

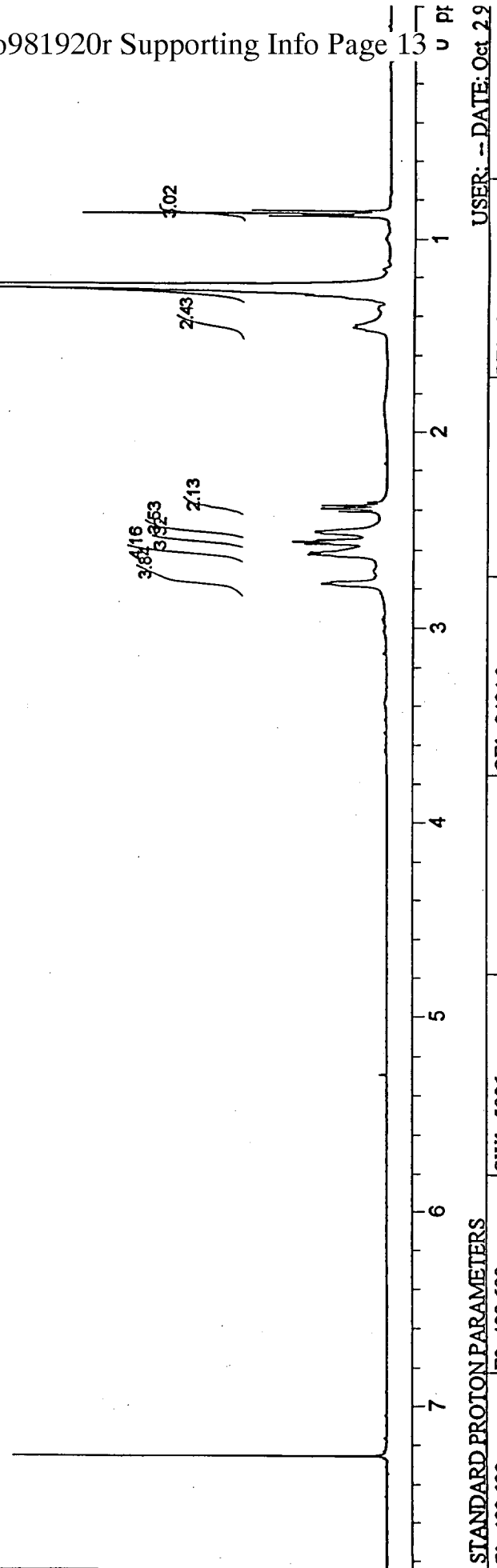
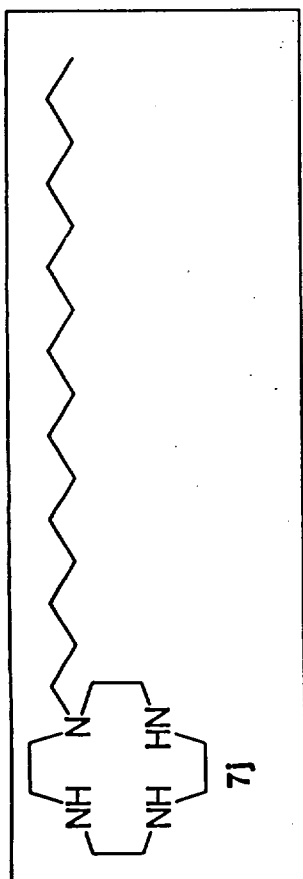
F2: 499.698

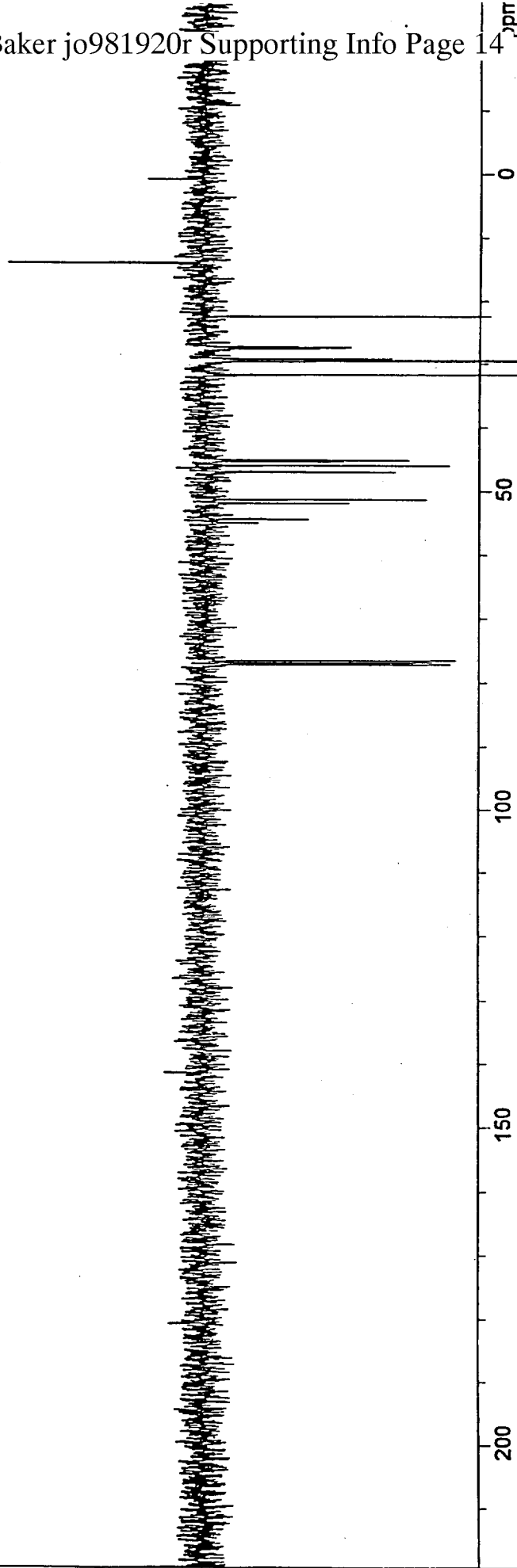
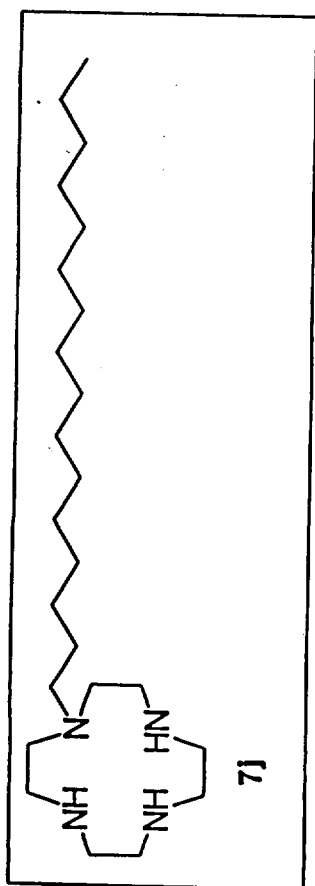
SW1: 30166

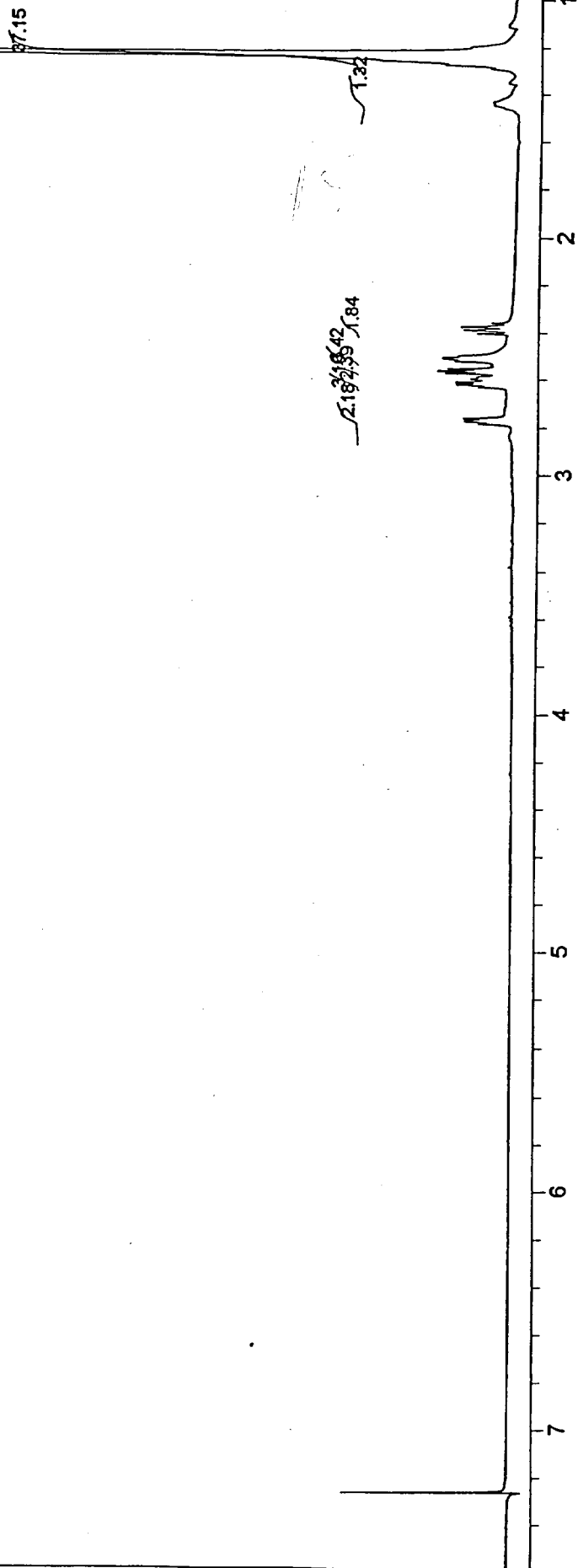
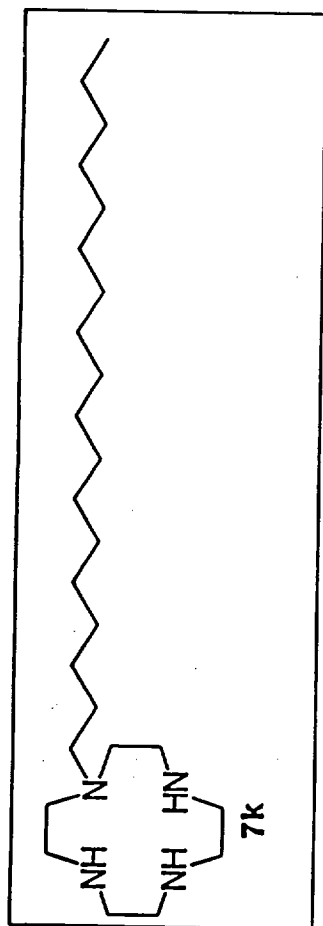
OF1: 13823.0

USER: -- DATE: Feb 19

0 pt







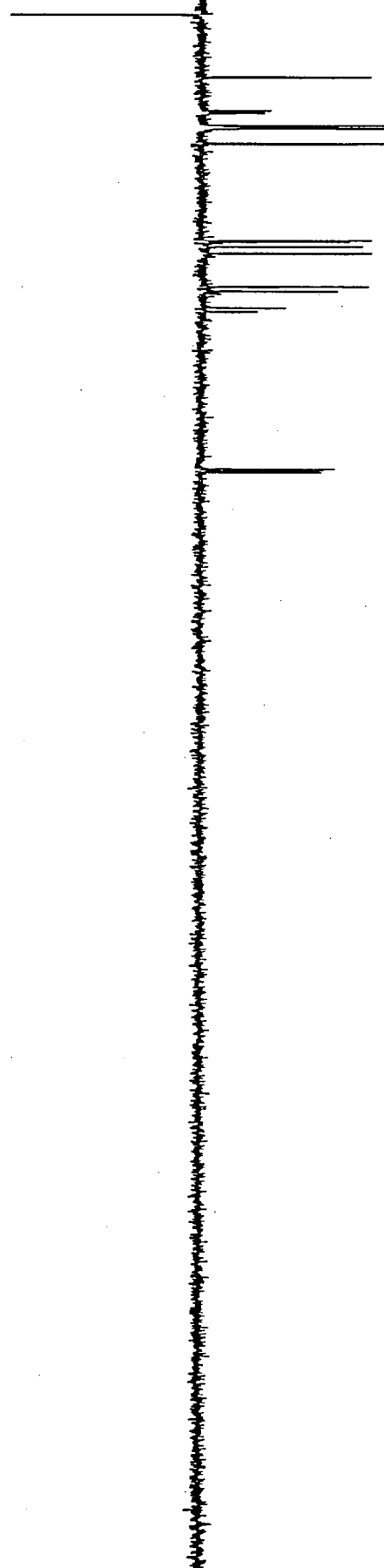
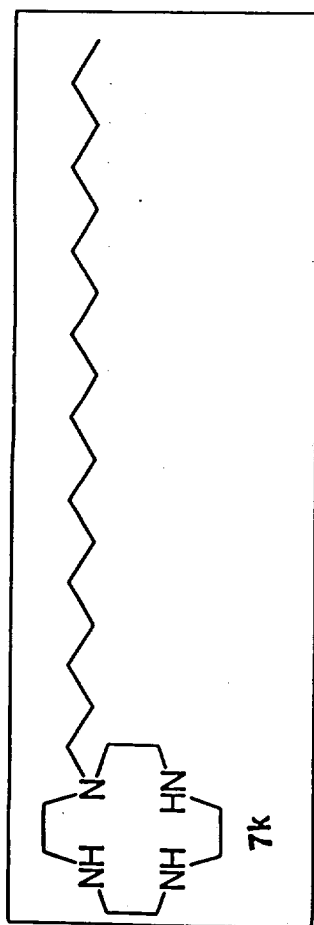
STANDARD PROTON PARAMETERS

F1: 400 600 F2: 400 600

SW1: 5006

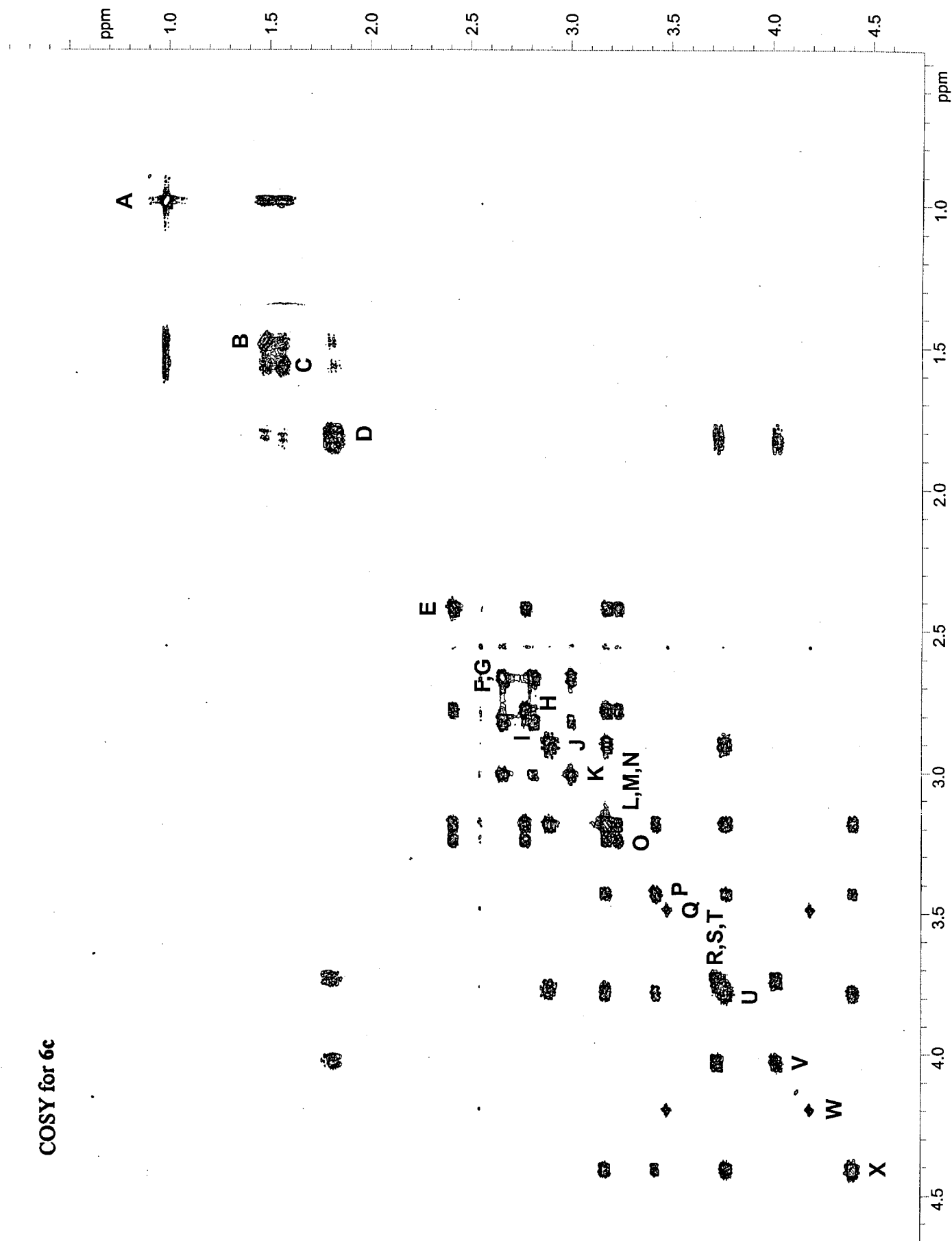
OE1: 24010

USER: -- DATE: Nov 26 97

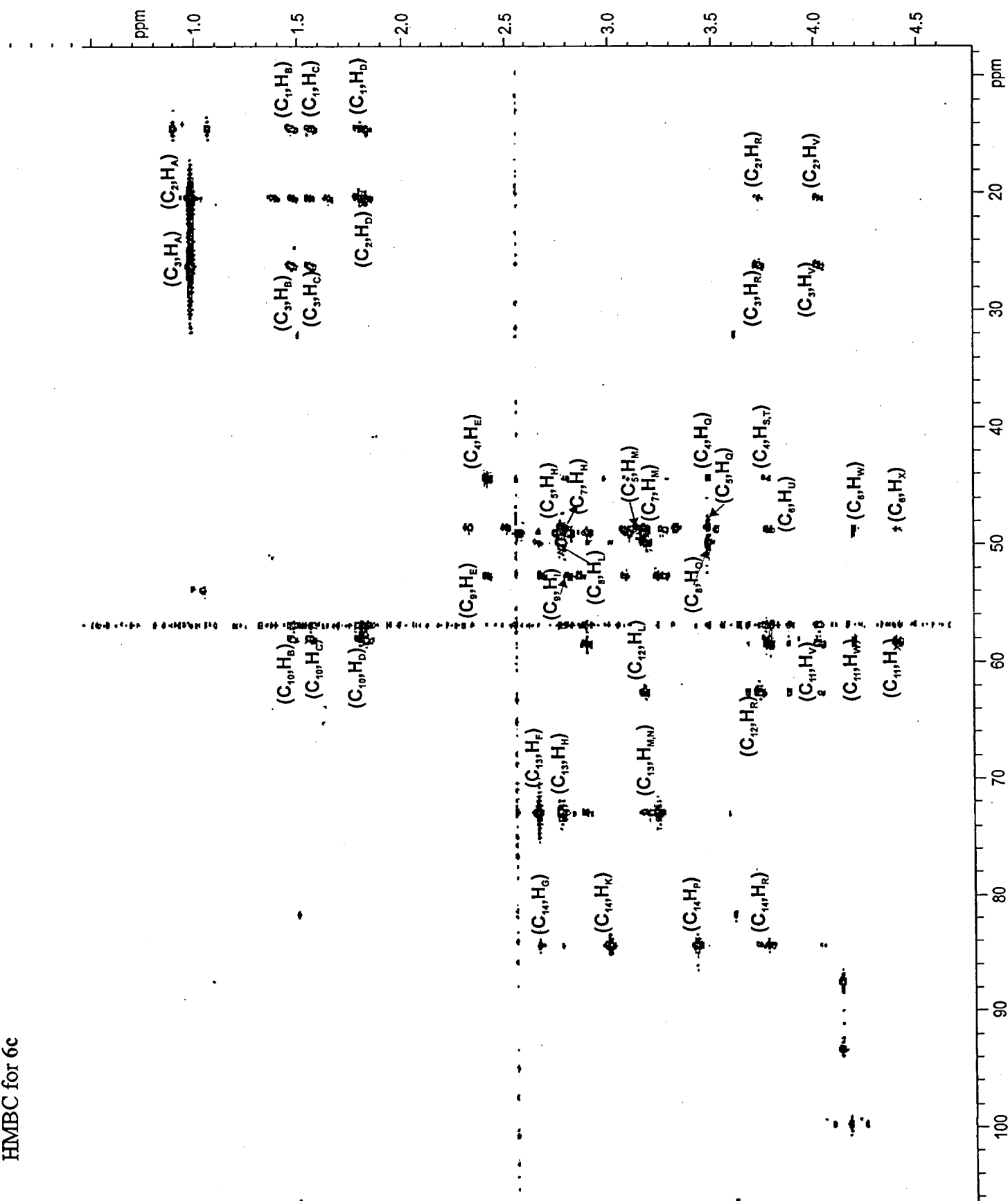


STANDARD CARBON PARAMETERS				0 pt...	USER: -- DATE: Jul 14 97
F1: 125.663	F2: 499.698	SW1: 30166	OF1: 13823.9	PTS1d: 32768	

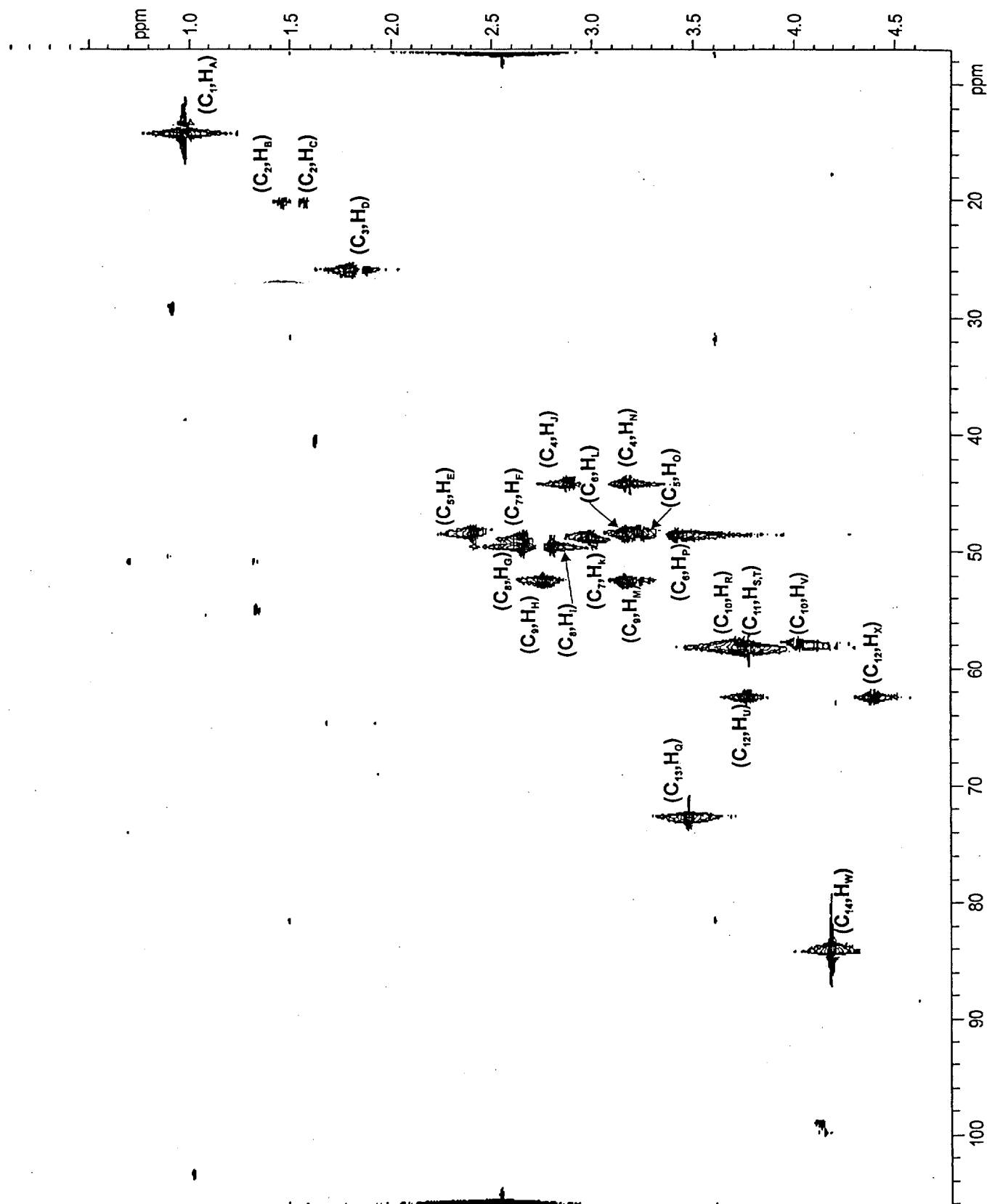
COSY for 6c

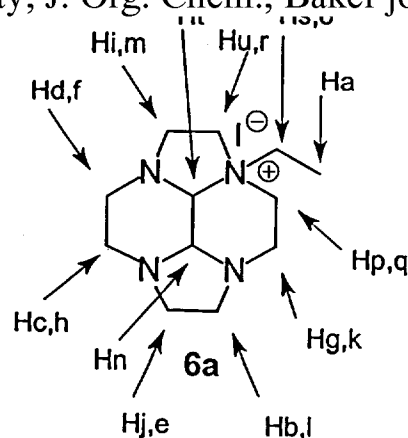


HMBC for 6c



HMQC for 6c

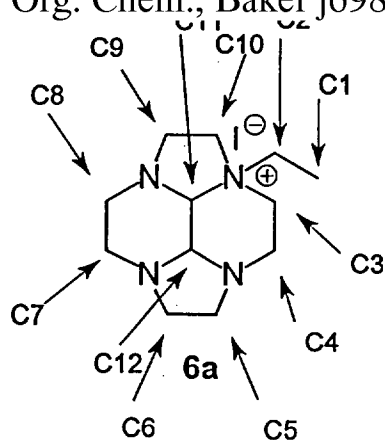




20

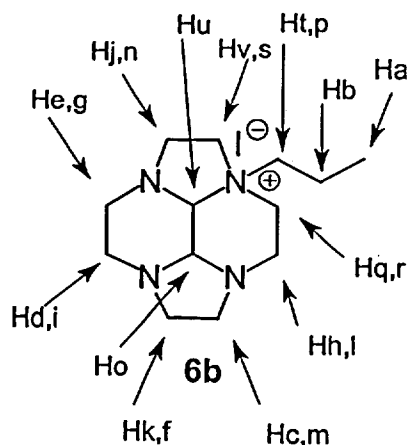
peak	δ , ppm	spin system	J, Hz	intensity	assignment
a	1.528	t	7.00	3	
b	2.434	ddd	J=10.20, 7.97, 6.30	1	
c	2.676	m		1	
d	2.704	m		1	
e	2.803	ddd	J=12.50, 8.03, 6.17	1	
f	2.848	td	J=12.20, 3.20	1	
g	2.925	ddd	J=13.20, 11.77, 2.34	1	
h	3.040	ddd	J=11.14, 3.07, 1.95	1	
i,j,k	3.200	m		3	
l	3.271	td	J=8.00, 4.53	1	
m	3.456	td	J=8.22, 2.58	1	
n	3.499	d	J=2.92	1	
o,p,q	3.781	m		3	
r	3.914	td	J=13.9, 7.26	1	
s	4.197	td	J=10.51, 6.34	1	
t	4.203	d	J=2.85	1	
u	4.434	ddd	J=11.60, 10.18, 3.06	1	

^1H NMR (500 MHz, CDCl_3) 1.528 (t, $J=7.00$ Hz, 3H) 2.434 (ddd, $J=10.20, 7.97, 6.30$ Hz, 1H), 2.676 (m, 1H), 2.704 (m, 1H) 2.803 (ddd, $J=12.50, 8.03, 6.17$ Hz, 1H) 2.848 (td, $J=12.20, 3.20$ Hz, 1H) 2.925 (ddd, $J=13.20, 11.77, 2.34$ Hz, 1H) 3.040 (ddd, $J=11.14, 3.07, 1.95$ Hz, 1H) 3.200 (m, 3H) 3.271 (td, $J=8.00, 4.53$ Hz, 1H) 3.456 (td, $J=8.22, 2.58$ Hz, 1H) 3.499 (d, $J=2.92$, 1H) 3.781 (m, 3H) 3.914 (td, $J=13.9, 7.26$ Hz, 1H) 4.197 (td, $J=10.51, 6.34$ Hz, 1H) 4.203 (d, $J=2.85$ Hz, 1H) 4.434 (ddd, $J=11.60, 10.18, 3.06$ Hz, 1H)



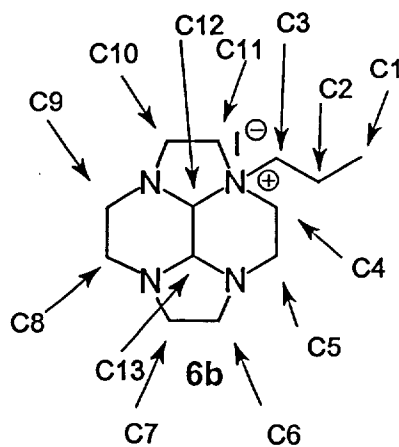
peak	δ , ppm	Simulat ed δ , ppm	mult.	assignment
I	9.43		CH ₃	C1, Me
II	43.695		CH ₂	C4 adjacent to N2 in 6 mem ring
III	47.906		CH ₂	C5, adjacent to N2 in 5 mem ring
IV	48.058		CH ₂	C9 adjacent to N4 on 5 mem ring
V	48.417		CH ₂	C7 adjacent to N3 on 6 mem ring
VI	49.147		CH ₂	C8 adjacent to N4 on 6 mem ring
VII	52.004		CH ₂	C6 adjacent to N3 on 5 mem ring
VIII	53.200		CH ₂	C2 on chain next to N ⁺
IX	57.304		CH ₂	C3 in 6 mem ring next to N1
X	61.428		CH ₂	C10 adjacent to N1 on 5 mem ring
XI	72.238		CH	C12 lower bridgehead carbon
XII	83.534		CH	C11 upper bridgehead carbon

¹³C NMR (500 MHz, CDCl₃) 9.43 43.695 47.906 48.058 48.417 49.147 52.004 53.200 57.304 61.428 72.238 83.534



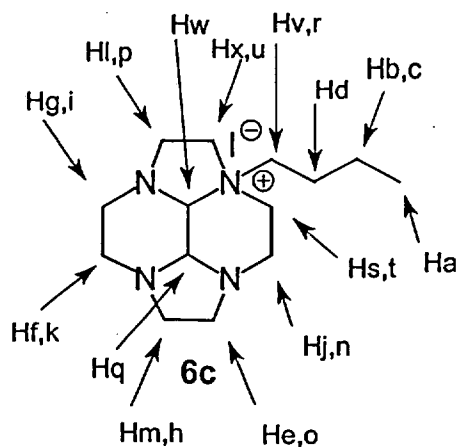
peak	δ , ppm	spin system	J, Hz	intensity	assignment
a	1.138	t	7.24	3	see assignments above
b	1.920	m		2	
c	2.442	ddd	J=9.33, 8.02, 5.90	1	
d	2.664	m		1	
e	2.696	m		1	
f	2.797	ddd	J=12.31, 8.03, 6.10	1	
g	2.838	td	J=11.13, 2.60	1	
h	2.936	ddd	J=13.63, 11.42, 2.52	1	
i	3.030	dt	J=12.10, 2.02	1	
j,k,l	3.193	m		3	
m	3.266	td	J=8.07, 4.60	1	
n	3.441	td	J=8.21, 2.52	1	
o	3.510	d	J=2.89	1	
p	3.747	td	J=12.50, 5.20	1	
q,r,s	3.800	m		3	
t	4.052	td	J=12.13, 5.13	1	
u	4.169	d	J=2.51	1	
v	4.516	ddd	J=12.40, 10.06, 2.89	1	

^1H NMR (500 MHz, CDCl_3) 1.138 (t, J=7.24 Hz, 3H) 1.920 (m, 2H) 2.442 (ddd, J=9.33, 8.02, 5.90 Hz, 1H) 2.664 (m, 1H) 2.696 (m, 1H) 2.797 (ddd, J=12.31, 8.03, 6.10 Hz, 1H) 2.838 (td, J=11.13, 2.60 Hz, 1H) 2.936 (ddd, J=13.63, 11.42, 2.52 Hz, 1H) 3.030 (dt, J=12.10, 2.02 Hz, 1H) 3.193 (m, 3H) 3.266 (td, J=8.07, 4.60 Hz, 1H) 3.441 (td, J=8.21, 2.52 Hz, 1H) 3.510 (d, J=2.89, 1H) 3.747 (td, J=12.50, 5.20, 1H) 3.800 (m, 3H) 4.052 (td, J=12.13, 5.13 Hz, 1H) 4.169 (d, J=2.51 Hz, 1H) 4.516 (ddd, J=12.40, 10.06, 2.89 Hz, 1H)



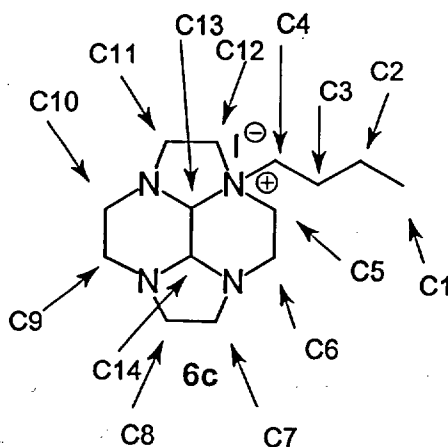
peak	δ , ppm	Simulat ed δ , ppm	mult.	assignment
I	10.956		CH ₃	C1, Me
II	17.313		CH ₂	C2, next to methyl
III	43.671		CH ₂	C5 adjacent to N2 in 6 mem ring
IV	47.843		CH ₂	C6, adjacent to N2 in 5 mem ring
V	48.125		CH ₂	C10 adjacent to N4 on 5 mem ring
VI	48.333		CH ₂	C8 adjacent to N3 on 6 mem ring
VII	49.168		CH ₂	C9 adjacent to N4 on 6 mem ring
VIII	52.016		CH ₂	C7 adjacent to N3 on 5 mem ring
IX	57.738		CH ₂	C3 on chain next to N ⁺
X	58.840		CH ₂	C4 in 6 mem ring next to N1
XI	62.024		CH ₂	C11 adjacent to N1 on 5 mem ring
XII	72.144		CH	C13 lower bridgehead carbon
XIII	83.614		CH	C12 upper bridgehead carbon

¹³C NMR (500 MHz, CDCl₃) 10.956 17.313 43.671 47.843 48.125 48.333 49.168 52.016 57.738 58.840 62.024 72.144 83.614



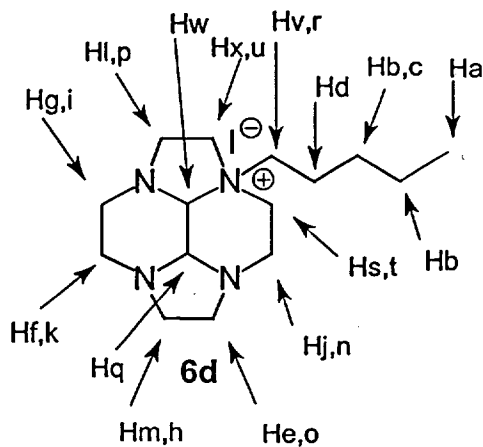
peak	δ , ppm	spin system	J, Hz	intensity	assignment
a	0.994	t	7.22	3	
b	1.491	m		1	
c	1.575	m		1	
d	1.827	m		2	
e	2.426	ddd	J=9.70, 8.18, 6.04	1	
f	2.664	m		1	
g	2.681	m		1	
h	2.786	ddd	J=12.50, 8.0, 5.91	1	
i	2.824	td	J=11.79, 2.86	1	
j	2.905	ddd	J=13.60, 10.5, 3.04	1	
k	3.013	ddd	J=13.60, 3.14, 1.91	1	
l,m,n	3.191	m		3	
o	3.247	td	J=8.18, 4.66	1	
p	3.430	td	J=8.2, 2.66	1	
q	3.490	d	J=2.93	1	
r	3.738	td	J=12.41, 5.37	1	
s,t,u	3.784	m		3	
v	4.030	td	J=12.24, 4.87	1	
w	4.199	d	J=2.81	1	
x	4.412	ddd	J=11.91, 10.15, 3.09	1	

^1H NMR (750 MHz, CDCl_3) 0.994 (t, J=7.22 Hz, 3H), 1.491 (m, 1H), 1.575 (m, 1H), 1.827 (m, 1H), 2.426 (ddd, J=9.70, 8.18, 6.04 Hz, 1H), 2.664 (m, 1H), 2.681 (m, 1H), 2.786 (ddd, J=12.50, 8.0, 5.91 Hz, 1H), 2.824 (td, J=11.79, 2.86 Hz, 1H), 2.905 (ddd, J=13.60, 10.5, 3.04 Hz, 1H), 3.013 (ddd, J=13.60, 3.14, 1.91 Hz, 1H), 3.191 (m, 3H), 3.247 (td, J=8.18, 4.66 Hz, 1H), 3.430 (td, J=8.2, 2.66 Hz, 1H), 3.490 (d, J=2.93, 1H), 3.738 (td, J=12.41, 5.37 Hz, 1H), 3.784 (m, 3H), 4.030 (td, J=12.24, 4.87 Hz, 1H), 4.199 (d, J=2.81 Hz, 1H), 4.412 (ddd, J=11.91, 10.15, 3.09 Hz, 1H)



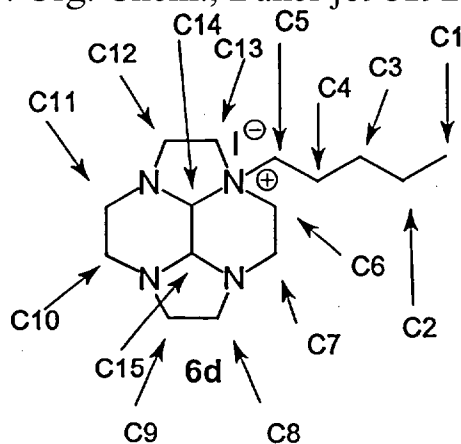
peak	δ , ppm	Simulat ed δ , ppm	mult.	assignment
I	13.799		CH ₃	C1, Me
II	19.760		CH ₂	C2 next to methyl
III	25.544		CH ₂	C3, chain carbon
VIII	43.685		CH ₂	C6 adjacent to N2 in 6 mem ring
IX	47.841		CH ₂	C7, adjacent to N2 in 5 mem ring
X	48.049		CH ₂	C11 adjacent to N4 on 5 mem ring
XI	48.327		CH ₂	C9 adjacent to N3 on 6 mem ring
XII	49.095		CH ₂	C10 adjacent to N4 on 6 mem ring
XIII	51.966		CH ₂	C8 adjacent to N3 on 5 mem ring
XIV	57.347		CH ₂	C4 on chain next to N+
XV	57.791		CH ₂	C5 in 6 mem ring next to N1
XVI	61.939		CH ₂	C12 adjacent to N1 on 5 mem ring
XVII	72.167		CH	C14 lower bridgehead carbon
XVIII	83.558		CH	C13 upper bridgehead carbon

¹³C NMR (500 MHz, CDCl₃) 13.799 19.760 25.544 43.685 47.841 48.049 48.327 49.095 51.966 57.347 57.791 61.939 72.167 83.558



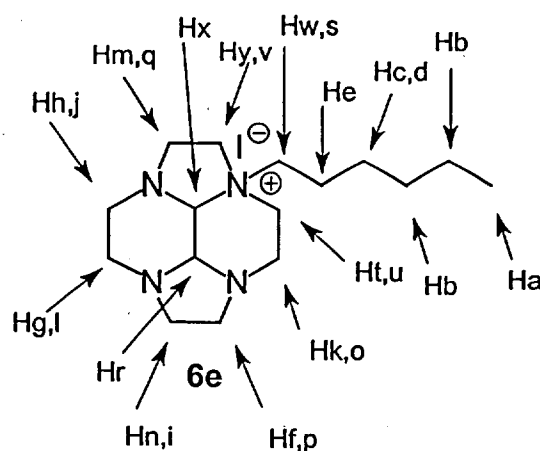
peak	δ , ppm	spin system	J, Hz	intensity	assignment
a	0.906	t	7.17	3	H1
b	1.404	m		3	H2
c	1.525	m		1	H4
d	1.840	m		2	H3
e	2.432	ddd	J=10.00, 8.19, 6.34	1	
f	2.668	m		1	benzyl methylene
g	2.707	m		1	
h	2.805	ddd	J=12.28, 8.16, 6.16	1	
i	2.826	td	J=12.60, 3.70	1	
j	2.889	ddd	J=13.69, 10.30, 4.97	1	
k	3.026	ddd	J=11.30, 2.70, 1.62	1	
l,m,n	3.201	m		3	
o	3.265	td	J=8.18, 4.68	1	
p	3.443	td	J=8.38, 2.81	1	
q	3.496	d	J=2.97	1	
r	3.745	ddd	J=13.00, 10.95, 6.68	1	
s,t,u	3.795	m		3	
v	4.043	td	J=10.76, 6.29	1	
w	4.220	d	J=2.86	1	
x	4.442	ddd	J=11.82, 10.04, 2.98	1	H2, benzyl methylenes

^1H NMR (750 MHz, CDCl_3) 0.906 (t, $J=7.17$ Hz, 3H) 1.404 (m, 3H) 1.525 (m, 1H), 1.840 (m, 1H) 2.432 (ddd, $J=10.00, 8.19, 6.34$ Hz, 1H), 2.668 (m, 1H), 2.707 (m, 1H) 2.805 (ddd, $J=12.28, 8.16, 6.16$ Hz, 1H) 2.826 (td, $J=12.60, 3.70$ Hz, 1H) 2.889 (ddd, $J=13.69, 10.30, 4.97$ Hz, 1H) 3.026 (ddd, $J=11.30, 2.70, 1.62$ Hz, 1H) 3.201 (m, 3H) 3.265 (td, $J=8.18, 4.68$ Hz, 1H) 3.443 (td, $J=8.38, 2.81$ Hz, 1H) 3.496 (d, $J=2.97$, 1H) 3.745 (ddd, $J=13.00, 10.95, 6.68$ Hz, 1H) 3.795 (m, 3H) 4.043 (td, $J=10.76, 6.29$ Hz, 1H) 4.220 (d, $J=2.86$ Hz, 1H) 4.442 (ddd, $J=11.82, 10.04, 2.98$ Hz, 1H)



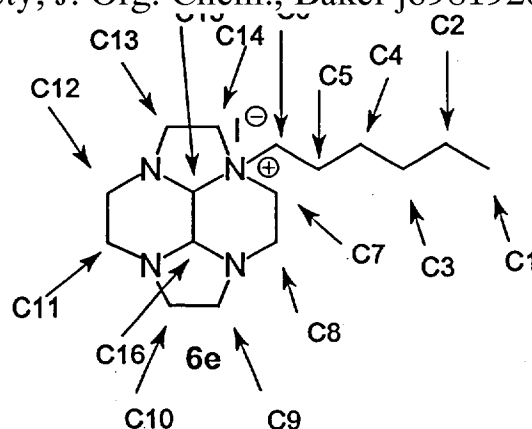
peak	δ , ppm	Simulat ed δ , ppm	mult.	assignment
I	13.856		CH ₃	C1, Me
II	22.377		CH ₃	C2 next to methyl
III	23.424		CH ₂	C3 chain carbon
IV	28.348		CH ₂	C4, chain carbon
V	43.745		CH ₂	C7 adjacent to N2 in 6 mem ring
VI	47.925		CH ₂	C8, adjacent to N2 in 5 mem ring
VII	48.146		CH ₂	C12 adjacent to N4 on 5 mem ring
VIII	48.325		CH ₂	C10 adjacent to N3 on 6 mem ring
IX	49.179		CH ₂	C11 adjacent to N4 on 6 mem ring
X	52.041		CH ₂	C9 adjacent to N3 on 5 mem ring
XI	57.521		CH ₂	C5 on chain next to N+
XII	57.850		CH ₂	C6 in 6 mem ring next to N1
XIII	61.997		CH ₂	C13 adjacent to N1 on 5 mem ring
XIV	72.285		CH	C15 lower bridgehead carbon
XV	83.501		CH	C14 upper bridgehead carbon

¹³C NMR (500 MHz, CDCl₃) 13.856 22.377 23.424 28.348 43.745 47.925 48.146 48.325 49.179 51.041 57.521 57.850 61.997 72.285 83.501



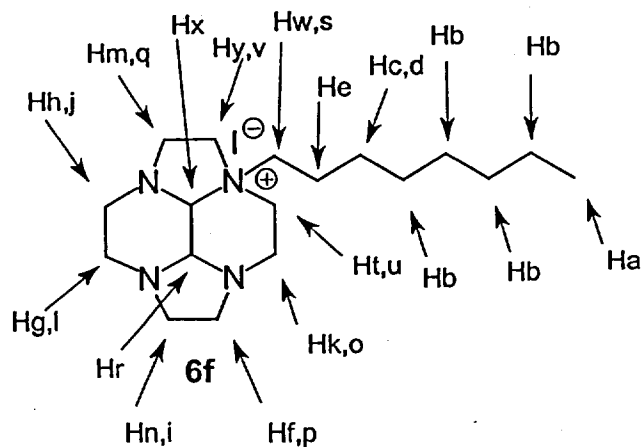
peak	δ , ppm	spin system	J, Hz	intensity	assignment
a	0.871	t	7.01	3	
b	1.328	m		4	
c	1.436	m		1	
d	1.547	m		1	
e	1.831	m		2	
f	2.419	ddd	J=9.86, 7.88, 5.96	1	
g	2.667	m		1	
h	2.701	m		1	
i	2.800	ddd	J=12.33, 8.03, 5.94	1	
j	2.830	td	J=11.10, 3.40	1	
k	2.872	ddd	J=13.75, 9.88, 4.02	1	
l	3.022	ddd	J=11.10, 3.36, 1.95	1	
m,n, o	3.198	m		3	
p	3.260	td	J=8.12, 4.69	1	
q	3.441	td	J=8.21, 2.86	1	
r	3.471	d	J=2.96	1	
s	3.730	ddd	J=12.88, 10.57, 8.28	1	
t,u,v	3.795	m		3	
w	4.051	td	J=12.81, 7.91	1	
x	4.208	d	J=2.85	1	
y	4.442	ddd	J=12.60, 9.96, 2.91	1	

^1H NMR (500 MHz, CDCl_3) 0.871 (t, J=7.01 Hz, 3H) 1.328 (m, 4H) 1.436 (m, 1H) 1.547 (m, 1H), 1.831 (m, 1H) 2.419 (ddd, J=9.86, 7.88, 5.96 Hz, 1H), 2.667 (m, 1H), 2.701 (m, 1H) 2.800 (ddd, J=12.33, 8.03, 5.94 Hz, 1H) 2.830 (td, J=11.10, 3.40 Hz, 1H) 2.872 (ddd, J=13.75, 9.88, 4.02 Hz, 1H) 3.022 (ddd, J=11.10, 3.36, 1.95 Hz, 1H) 3.198 (m, 3H) 3.260 (td, J=8.12, 4.69 Hz, 1H) 3.441 (td, J=8.21, 2.86 Hz, 1H) 3.471 (d, J=2.96, 1H) 3.730 (ddd, J=12.88, 10.57, 8.28 Hz, 1H) 3.795 (m, 3H) 4.051 (td, J=12.81, 7.91 Hz, 1H) 4.208 (d, J=2.85 Hz, 1H) 4.442 (ddd, J=12.60, 9.96, 2.91 Hz, 1H)



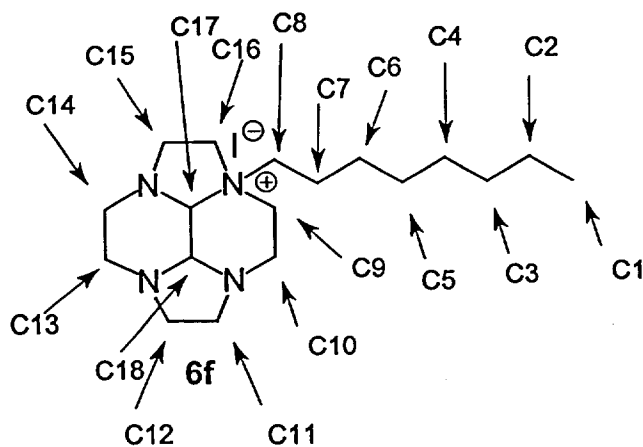
peak	δ , ppm	Simulat ed δ , ppm	mult.	assignment
I	13.900		CH ₃	C1, Me
II	22.317		CH ₂	C2, next to methyl
III	23.612		CH ₂	C3, chain carbon
IV	25.977		CH ₂	C4, chain carbon
V	31.275		CH ₂	C5, chain carbon
VI	43.683		CH ₂	C8 adjacent to N2 in 6 mem ring
VII	47.863		CH ₂	C9, adjacent to N2 in 5 mem ring
VIII	48.085		CH ₂	C13 adjacent to N4 on 5 mem ring
IX	48.330		CH ₂	C11 adjacent to N3 on 6 mem ring
X	49.098		CH ₂	C12 adjacent to N4 on 6 mem ring
XI	51.974		CH ₂	C10 adjacent to N3 on 5 mem ring
XII	57.467		CH ₂	C6 on chain next to N ⁺
XIII	57.808		CH ₂	C7 in 6 mem ring next to N1
XIV	61.940		CH ₂	C14 adjacent to N1 on 5 mem ring
XV	72.230		CH ₂	C16 lower bridgehead carbon
XVI	83.430		CH ₂	C15 upper bridgehead carbon

¹³C NMR (500 MHz, CDCl₃) 13.900 22.317 23.612 25.977 31.275 43.683 47.863 48.085 48.330 49.098 51.974 57.467 57.808 61.940 72.230 83.430



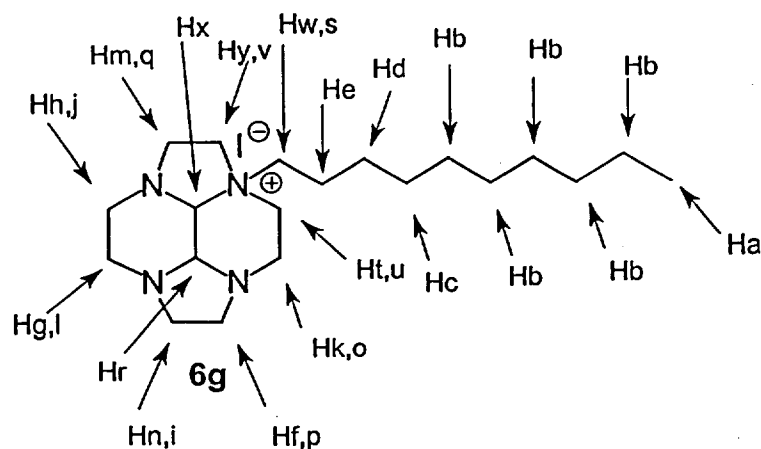
peak	δ , ppm	spin system	J, Hz	intensity	assignment
a	0.849	t	7.12	3	see assignments above
b	1.304	m		8	
c	1.436	m		1	
d	1.518	m		1	
e	1.823	m		2	
f	2.459	ddd	J=10.47, 8.32, 4.41	1	
g	2.684	m		1	
h	2.718	m		1	
i	2.800	ddd	J=13.95, 8.09, 3.45	1	
j	2.862	td	J=11.10, 3.20	1	
k	2.910	ddd	J=11.55, 8.75, 4.00	1	
l	3.032	ddd	J=10.88, 3.34, 2.03	1	
m,n, o	3.212	m		3	
p	3.273	td	J=8.08, 4.86	1	
q	3.453	td	J=8.40, 2.98	1	
r	3.550	d	J=2.85	1	
s	3.744	ddd	J=13.03, 10.03, 7.02	1	
t,u,v	3.794	m		3	
w	4.026	td	J=12.78, 7.94	1	
x	4.235	d	J=2.81	1	
y	4.404	ddd	J=12.01, 9.96, 3.06	1	

^1H NMR (500 MHz, CDCl_3) 0.849 (t, J=7.12 Hz, 3H) 1.304 (m, 8H) 1.436 (m, 1H) 1.518 (m, 1H), 1.823 (m, 2H) 2.459 (ddd, J=10.47, 8.32, 4.41 Hz, 1H), 2.684 (m, 1H), 2.718 (m, 1H) 2.800 (ddd, J=13.95, 8.09, 3.45 Hz, 1H) 2.862 (td, J=11.10, 3.20 Hz, 1H) 2.910 (ddd, J=11.55, 8.75, 4.00 Hz, 1H) 3.032 (ddd, J=10.88, 3.34, 2.03 Hz, 1H) 3.212 (m, 3H) 3.273 (td, J=8.08, 4.86 Hz, 1H) 3.453 (td, J=8.40, 2.98 Hz, 1H) 3.550 (d, J=2.85, 1H) 3.744 (ddd, J=13.03, 10.03, 7.02 Hz, 1H) 3.795 (m, 3H) 4.026 (td, J=12.78, 7.94 Hz, 1H) 4.235 (d, J=2.81 Hz, 1H) 4.404 (ddd, J=12.01, 9.96, 3.06 Hz, 1H)



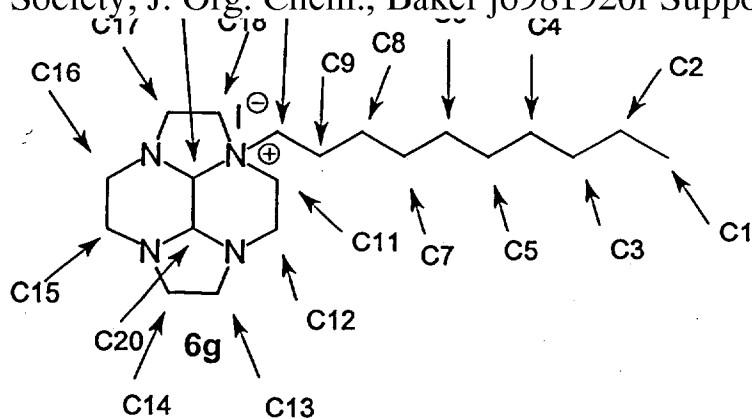
peak	δ , ppm	Simulat ed δ , ppm	mult.	assignment
I	14.019		CH ₃	C1, Me
II	22.531		CH ₂	C2, next to methyl
III	23.694		CH ₂	C3, chain carbon
IV	26.345		CH ₂	C4, chain carbon
V	28.976		CH ₂	C5, chain carbon
VI	29.207		CH ₂	C6, chain carbon
VII	31.630		CH ₂	C7, chain carbon
VIII	43.696		CH ₂	C10 adjacent to N2 in 6 mem ring
IX	47.899		CH ₂	C11, adjacent to N2 in 5 mem ring
X	48.111		CH ₂	C15 adjacent to N4 on 5 mem ring
XI	48.354		CH ₂	C13 adjacent to N3 on 6 mem ring
XII	49.114		CH ₂	C14 adjacent to N4 on 6 mem ring
XIII	51.981		CH ₂	C12 adjacent to N3 on 5 mem ring
XIV	57.466		CH ₂	C8 on chain next to N ⁺
XV	57.847		CH ₂	C9 in 6 mem ring next to N1
XVI	61.959		CH ₂	C16 adjacent to N1 on 5 mem ring
XVII	72.255		CH	C18 lower bridgehead carbon
XVIII	83.421		CH	C17 upper bridgehead carbon

¹³C NMR (500 MHz, CDCl₃) 14.019 22.531 23.694 26.345 28.976 29.207 31.630 43.696 47.899 48.111 48.354 49.114 51.981 57.466 57.847 57.847 61.959 72.255 83.421



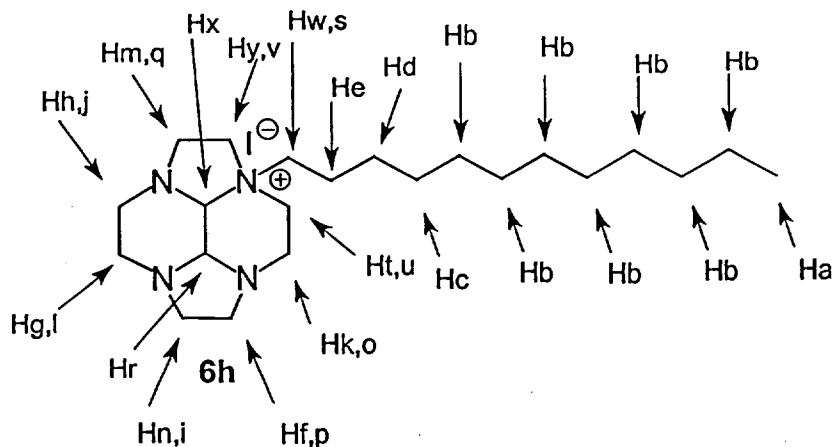
peak	δ , ppm	spin system	J, Hz	intensity	assignment
a	0.864	t	7.09	3	
b	1.247	m		10	
c	1.352	m		2	
d	1.490	m		2	
e	1.824	m		2	
f	2.432	ddd	J=9.74, 8.01, 5.62	1	
g	2.686	m		1	
h	2.715	m		1	
i	2.824	ddd	J=12.48, 8.11, 5.91	1	
j	2.862	td	J=11.71, 2.80	1	
k	2.881	ddd	J=13.93, 8.40, 5.97	1	
l	3.043	ddd	J=11.12, 4.76, 1.94	1	
m,n, o	3.205	m		3	
p	3.278	td	J=8.25, 4.62	1	
q	3.459	td	J=8.21, 2.89	1	
r	3.498	d	J=2.78	1	
s	3.754	ddd	J=12.78, 10.30, 7.06	1	
t,u,v	3.798	m		3	
w	4.052	td	J=12.91, 5.83	1	
x	4.228	d	J=2.90	1	
y	4.443	ddd	J=12.96, 10.12, 3.03	1	

^1H NMR (500 MHz, CDCl_3) 0.864 (t, J=7.09 Hz, 3H) 1.247 (m, 10H) 1.352 (m, 2H) 1.490 (m, 2H), 1.824 (m, 2H) 2.432 (ddd, J=9.74, 8.01, 5.62 Hz, 1H), 2.686 (m, 1H), 2.715 (m, 1H) 2.824 (ddd, J=12.48, 8.11, 5.91 Hz, 1H) 2.862 (td, J=11.71, 2.80 Hz, 1H) 2.881 (ddd, J=13.93, 8.40, 5.97 Hz, 1H) 3.043 (ddd, J=11.12, 4.76, 1.94 Hz, 1H) 3.205 (m, 3H) 3.278 (td, J=8.25, 4.62 Hz, 1H) 3.459 (td, J=8.21, 2.89 Hz, 1H) 3.498 (d, J=2.78, 1H) 3.754 (ddd, J=12.78, 10.030, 7.06 Hz, 1H) 3.798 (m, 3H) 4.052 (td, J=12.91, 5.83 Hz, 1H) 4.228 (d, J=2.90 Hz, 1H) 4.443 (ddd, J=12.96, 10.12, 3.03 Hz, 1H)



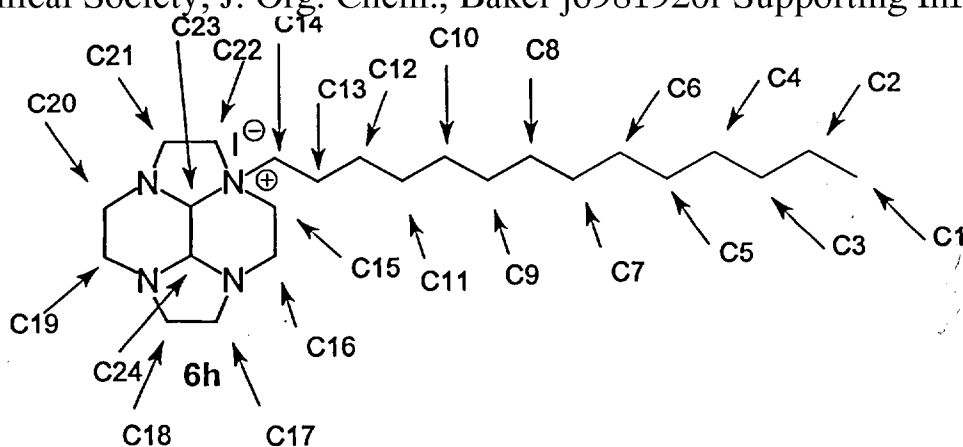
peak	δ , ppm	Simulat ed δ , ppm	mult.	assignment
I	14.015		CH ₃	C1, Me
II	22.551		CH ₂	C2, next to methyl
III	23.637		CH ₂	C3, chain carbon
IV	26.335		CH ₂	C4, chain carbon
V	29.170		CH ₂	C5, chain carbon
VI	29.212		CH ₂	C6, chain carbon
VII	29.302		CH ₂	C7, chain carbon
VIII	29.377		CH ₂	C8, chain carbon
IX	31.734		CH ₂	C9, chain carbon
X	43.651		CH ₂	C12 adjacent to N2 in 6 mem ring
XI	47.830		CH ₂	C13, adjacent to N2 in 5 mem ring
XII	48.015		CH ₂	C17 adjacent to N4 on 5 mem ring
XIII	48.246		CH ₂	C15 adjacent to N3 on 6 mem ring
XIV	49.056		CH ₂	C16 adjacent to N4 on 6 mem ring
XV	51.921		CH ₂	C14 adjacent to N3 on 5 mem ring
XVI	57.563		CH ₂	C10 on chain next to N+
XVII	57.714		CH ₂	C11 in 6 mem ring next to N1
XVIII	61.956		CH ₂	C18 adjacent to N1 on 5 mem ring
XIV	72.120		CH	C20 lower bridgehead carbon
XV	83.350		CH	C19 upper bridgehead carbon

¹³C NMR (500 MHz, CDCl₃) 14.015 22.551 23.637 26.335 29.170 29.212 29.302 29.377 31.734 43.651 47.830 48.015 48.246 49.056 51.921 57.563 57.714 61.956 72.120 83.350



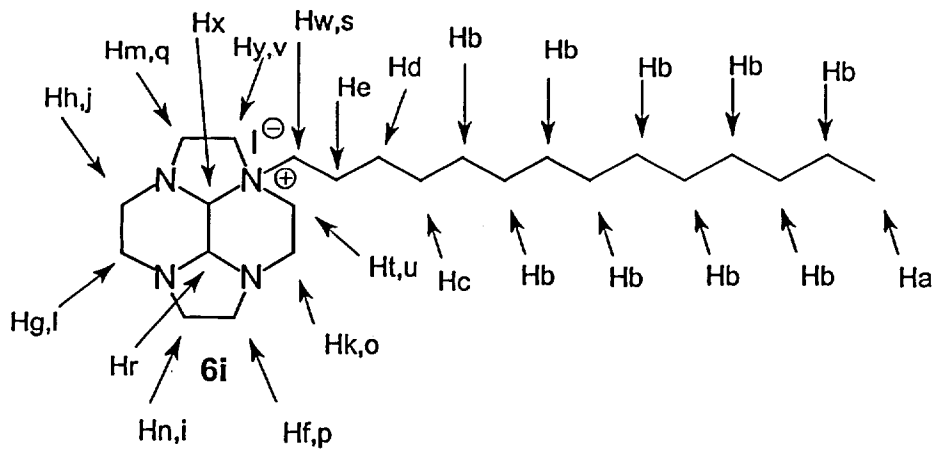
peak	δ , ppm	spin system	J, Hz	intensity	assignment
a	0.874	t	7.11	3	
b	1.251	m		14	
c	1.360	m		2	
d	1.500	m		2	
e	1.816	m		2	
f	2.411	ddd	J=9.66, 7.70, 5.45	1	
g	2.690	m		1	
h	2.722	m		1	
i	2.821	ddd	J=12.04, 8.22, 6.17	1	
j	2.837	td	J=11.78, 2.97	1	
k	2.850	ddd	J=12.30, 8.62, 5.33	1	
l	3.043	ddd	J=11.33, 4.55, 1.66	1	
m,n, o	3.216	m		3	
p	3.286	td	J=8.16, 4.79	1	
q	3.447	td	J=9.07, 3.22	1	
r	3.450	d	J=2.86	1	
s	3.760	td	J=12.92, 5.64	1	
t,u,v	3.806	m		3	
w	4.108	td	J=12.05, 5.18	1	
x	4.224	d	J=2.86	1	
y	4.443	ddd	J=12.34, 9.99, 3.24	1	

^1H NMR (500 MHz, CDCl_3) 0.874 (t, J=7.11 Hz, 3H) 1.251 (m, 14H) 1.360 (m, 2H) 1.500 (m, 2H), 1.816 (m, 2H) 2.411 (ddd, J=9.66, 7.70, 5.45 Hz, 1H), 2.690 (m, 1H), 2.722 (m, 1H) 2.821 (ddd, J=12.04, 8.22, 6.17 Hz, 1H) 2.837 (td, J=11.78, 2.97 Hz, 1H) 2.850 (ddd, J=12.30, 8.62, 5.33 Hz, 1H) 3.043 (ddd, J=11.33, 4.55, 1.66 Hz, 1H) 3.216 (m, 3H) 3.286 (td, J=8.16, 4.79 Hz, 1H) 3.447 (td, J=9.07, 3.22 Hz, 1H) 3.450 (d, J=2.86, 1H) 3.760 (td, J=12.92, 5.64 Hz, 1H) 3.806 (m, 3H) 4.108 (td, J=12.05, 5.18 Hz, 1H) 4.224 (d, J=2.86 Hz, 1H) 4.443 (ddd, J=12.34, 9.99, 3.24 Hz, 1H)



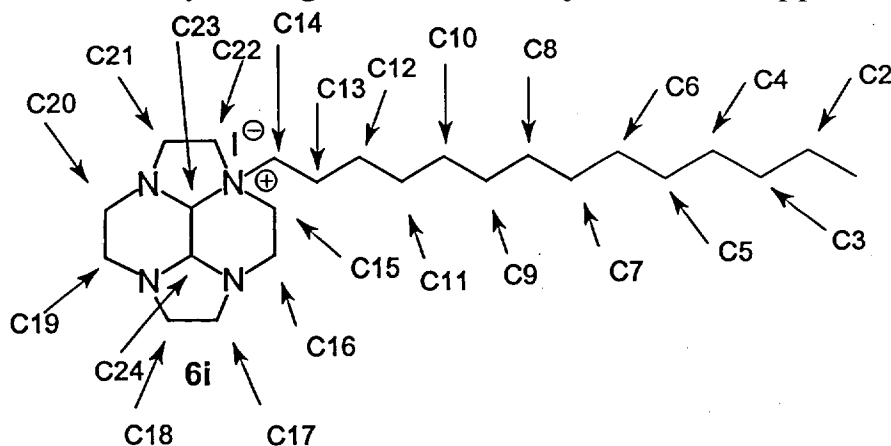
peak	δ , ppm	Simulat ed δ , ppm	mult.	assignment
I	14.109		CH ₃	C1, Me
II	17.304		CH ₂	C2 next to methyl
III	22.672		CH ₂	C3 chain carbon
IV	23.744		CH ₂	C4, chain carbon
V	26.394		CH ₂	C5, chain carbon
VI	29.333		CH ₂	C6, chain carbon
VII	29.361		CH ₂	C7, chain carbon
VIII	29.510		CH ₂	C8, chain carbon
IX	29.585		CH ₂	C9,C10 chain carbons
X	31.893		CH ₂	C11, chain carbon
XI	43.762		CH ₂	C14 adjacent to N2 in 6 mem ring
XII	47.996		CH ₂	C15, adjacent to N2 in 5 mem ring
XIII	48.217		CH ₂	C19 adjacent to N4 on 5 mem ring
XIV	48.434		CH ₂	C17 adjacent to N3 on 6 mem ring
XV	49.170		CH ₂	C18 adjacent to N4 on 6 mem ring
XVI	52.037		CH ₂	C16 adjacent to N3 on 5 mem ring
XVII	57.460		CH ₂	C12 on chain next to N ⁺
XVIII	58.005		CH ₂	C13 in 6 mem ring next to N1
XIV	62.041		CH ₂	C20 adjacent to N1 on 5 mem ring
XV	72.397		CH	C22 lower bridgehead carbon
XVI	83.368		CH	C21 upper bridgehead carbon

¹³C NMR (500 MHz, CDCl₃) 14.109 17.304 22.672 23.744 26.394 29.333 29.361 29.510 29.585 31.893 43.762 47.996 48.217 48.434 49.170 52.037 57.460 58.005 62.041 72.397 83.368



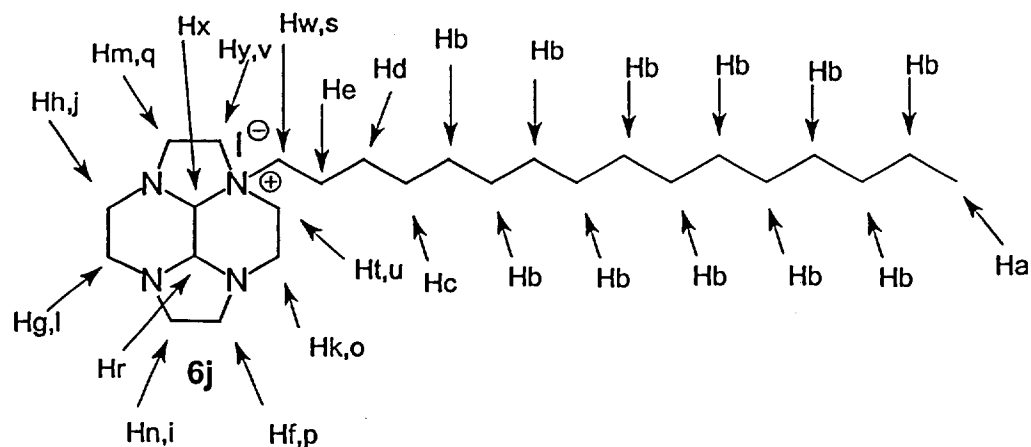
peak	δ , ppm	spin system	J, Hz	intensity	assignment
a	0.870	t	7.13	3	
b	1.243	m		18	
c	1.356	m		2	
d	1.494	m		2	
e	1.812	m		2	
f	2.405	ddd	J=9.46, 7.96, 5.69	1	
g	2.692	m		1	
h	2.716	m		1	
I	2.818	ddd	J=12.31, 7.93, 5.99	1	
j	2.831	td	J=10.78, 2.93	1	
k	2.853	ddd	J=12.89, 9.63, 5.92	1	
l	3.045	ddd	J=11.44, 5.13, 1.92	1	
m,n, o	3.205	m		3	
p	3.288	td	J=8.28, 4.78	1	
q	3.445	d	J=2.95	1	
r	3.452	td	J=8.09, 2.53	1	
s	3.751	td	J=12.79, 4.91	1	
t,u,v	3.802	m		3	
w	4.087	td	J=12.66, 4.90	1	
x	4.224	d	J=2.71	1	
y	4.443	ddd	J=13.20, 10.03, 3.18	1	

¹H NMR (500 MHz, CDCl₃) 0.870 (t, J=7.13 Hz, 3H) 1.243 (m, 18H) 1.356 (m, 2H) 1.494 (m, 2H), 1.812 (m, 2H) 2.405 (ddd, J=9.46, 7.96, 5.69 Hz, 1H), 2.692 (m, 1H), 2.716 (m, 1H) 2.818 (ddd, J=12.31, 7.93, 5.99 Hz, 1H) 2.831 (td, J=10.78, 2.93 Hz, 1H) 2.853 (ddd, J=12.89, 9.63, 5.92 Hz, 1H) 3.045 (ddd, J=11.44, 5.13, 1.92 Hz, 1H) 3.205 (m, 3H) 3.288 (td, J=8.28, 4.78 Hz, 1H) 3.445 (d, J=2.95 Hz, 1H) 3.452 (td, J=8.09, 2.53 Hz, 1H) 3.751 (td, J=12.79, 4.91 Hz, 1H) 3.802 (m, 3H) 4.087 (td, J=12.66, 4.90 Hz, 1H) 4.224 (d, J=2.71 Hz, 1H) 4.443 (ddd, J=13.20, 10.03, 3.18 Hz, 1H)



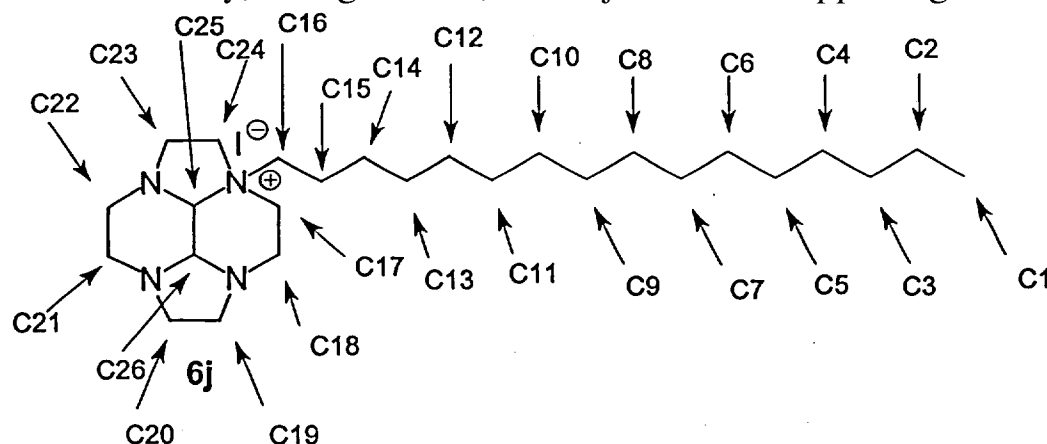
peak	δ , ppm	Simulat ed δ , ppm	mult.	assignment
I	14.122		CH ₃	C1, Me
II	22.681		CH ₂	C2 next to methyl
III	23.743		CH ₂	C3 chain carbon
IV	26.424		CH ₂	C4, chain carbon
V	28.525		CH ₂	C5, chain carbon
VI	29.356		CH ₂	C6, chain carbon
VII	29.391		CH ₂	C7, chain carbon
VIII	29.458		CH ₂	C8, chain carbon
IX	29.547		CH ₂	C9 chain carbons
X	29.651		CH ₂	C10,11, chain carbon
XI	29.684		CH ₂	C12, chain carbon
XII	31.911		CH ₂	C13, chain carbon
XIII	43.709		CH ₂	C16 adjacent to N2 in 6 mem ring
XIV	47.908		CH ₂	C17, adjacent to N2 in 5 mem ring
XV	48.186		CH ₂	C21 adjacent to N4 on 5 mem ring
XVI	48.363		CH ₂	C19 adjacent to N3 on 6 mem ring
XVII	49.169		CH ₂	C20 adjacent to N4 on 6 mem ring
XVIII	52.043		CH ₂	C18 adjacent to N3 on 5 mem ring
XIV	57.582		CH ₂	C14 on chain next to N ⁺
XV	57.879		CH ₂	C15 in 6 mem ring next to N1
XVI	62.064		CH ₂	C22 adjacent to N1 on 5 mem ring
XVII	72.256		CH	C24 lower bridgehead carbon
XVIII	83.353		CH	C23 upper bridgehead carbon

¹³C NMR (500 MHz, CDCl₃) 14.122 22.681 23.743 26.424 28.525 29.356 29.391 29.458 29.547 29.651 29.684 31.911 43.709 47.908 48.186 48.363 49.169 52.043 57.582 62.064 72.256 83.353



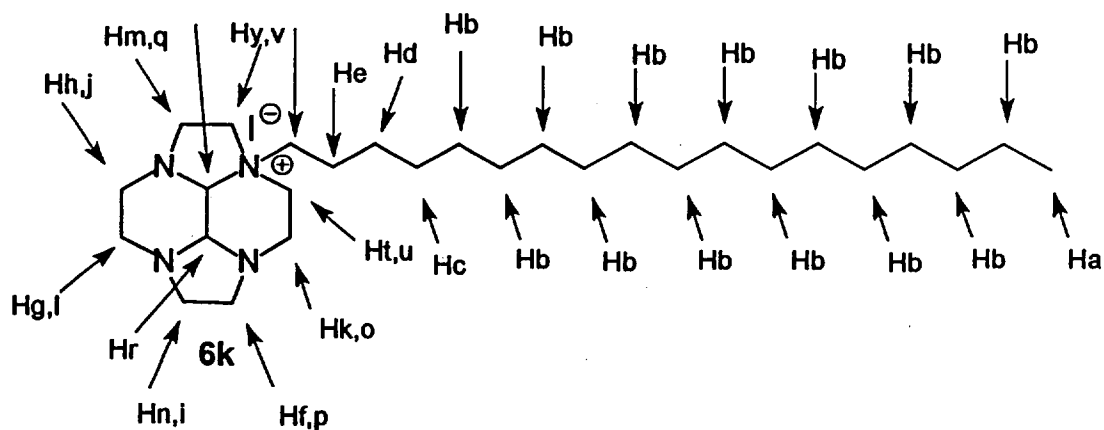
peak	δ , ppm	spin system	J, Hz	intensity	assignment
a	0.865	t	7.11	3	See drawing for all assignments
b	1.254	m		22	
c	1.351	m		2	
d	1.486	m		2	
e	1.813	m		2	
f	2.415	ddd	J=9.59, 7.91, 5.79	1	
g	2.686	m		1	
h	2.716	m		1	
i	2.818	ddd	J=12.98, 8.01, 5.96	1	
j	2.832	m		1	
k	2.860	ddd	J=12.89, 9.63, 6.69	1	
l	3.038	ddd	J=11.00, 4.56, 2.03	1	
m,n, o	3.196	m		3	
p	3.278	td	J=8.04, 4.55	1	
q	3.452	td	J=8.18, 2.66	1	
r	3.467	d	J=2.81	1	
s	3.755	td	J=11.43, 6.04	1	
t,u,v	3.801	m		3	
w	4.087	td	J=12.52, 5.08	1	
x	4.225	d	J=2.68	1	
y	4.443	ddd	J=12.11, 10.03, 3.32	1	

^1H NMR (500 MHz, CDCl_3) 0.865 (t, J=7.11 Hz, 3H) 1.254 (m, 22H) 1.351 (m, 2H) 1.486 (m, 2H) 1.813 (m, 2H) 2.415 (ddd, J=9.59, 7.91, 5.79 Hz, 1H) 2.686 (m, 1H) 2.716 (m, 1H) 2.818 (ddd, J=12.98, 9.63, 6.69 Hz, 1H) 2.832 (m, 1H) 2.860 (ddd, J=12.89, 9.63, 6.69 Hz, 1H) 3.038 (ddd, J=11.00, 4.56, 2.03 Hz, 1H) 3.196 (m, 3H) 3.278 (td, J=8.04, 4.55 Hz, 1H) 3.452 (td, J=8.18, 2.66 Hz, 1H) 3.467 (d, J=2.81 Hz, 1H) 3.755 (td, J=11.43, 6.04 Hz, 1H) 3.801 (m, 3H) 4.087 (td, J=12.52, 5.08 Hz, 1H) 4.225 (d, J=2.68 Hz, 1H) 4.443 (ddd, J=12.11, 10.03, 3.32 Hz, 1H)



peak	δ , ppm	Simulat ed δ , ppm	mult.	assignment
I	14.095		CH ₃	C1, Me
II	22.664		CH ₂	C2, next to methyl
III	23.717		CH ₂	C3, chain carbon
IV	26.368		CH ₂	C4, chain carbon
V	29.345		CH ₂	C5, C6, C7 chain carbons
VI	29.505		CH ₂	C8, chain carbon
VII	29.593		CH ₂	C9, chain carbon
VIII	29.628		CH ₂	C10, C11, chain carbons
IX	29.672		CH ₂	C12, C13, C14 chain carbons
X	31.891		CH ₂	C15, chain carbon
XI	43.743		CH ₂	C18 adjacent to N2 in 6 mem ring
XII	47.978		CH ₂	C19, adjacent to N2 in 5 mem ring
XIII	48.196		CH ₂	C17 adjacent to N4 on 5 mem ring
XIV	48.421		CH ₂	C21 adjacent to N3 on 6 mem ring
XV	49.145		CH ₂	C22 adjacent to N4 on 6 mem ring
XVI	52.013		CH ₂	C20 adjacent to N3 on 5 mem ring
XVII	57.425		CH ₂	C16 on chain next to N+
XVIII	57.974		CH ₂	C23 in 6 mem ring next to N1
XIV	62.023		CH ₂	C24 adjacent to N1 on 5 mem ring
XV	72.375		CH	C26 lower bridgehead carbon
XVI	83.338		CH	C25 upper bridgehead carbon

¹³C NMR (500 MHz, CDCl₃) 14.095 22.664 23.717 26.368 29.345 29.505 29.593 29.628 29.672 31.891 43.743 47.978 48.196 48.421 49.145 52.013 57.425 57.974 62.023 72.375 83.338



peak	δ , ppm	spin system	J, Hz	intensity	assignment
a	0.864	t	7.12	3	See drawing for all assignments
b	1.241	m		26	
c	1.351	m		2	
d	1.488	m		2	
e	1.813	m		2	
f	2.420	ddd	J=9.62, 7.23, 5.70	1	
g	2.682	m		1	
h	2.719	m		1	
i	2.814	ddd	J=12.02, 7.93, 5.96	1	
j	2.838	m		1	
k	2.874	ddd	J=13.44, 9.58, 6.72	1	
l	3.039	td	J=11.30, 2.36	1	
m,n, o	3.196	m		3	
p	3.269	td	J=8.05, 4.62	1	
q	3.453	td	J=8.24, 2.64	1	
r	3.474	d	J=2.76	1	
s	3.743	td	J=11.20, 5.63	1	
t,u,v	3.797	m		3	
w	4.087	td	J=11.18, 5.18	1	
x	4.226	d	J=2.88	1	
y	4.443	ddd	J=11.82, 10.24, 2.80	1	

^1H NMR (500 MHz, CDCl_3) 0.864 (t, J=7.12 Hz, 3H) 1.241 (m, 26H) 1.351 (m, 2H) 1.488 (m, 2H), 1.813 (m, 2H) 2.420 (ddd, J=9.62, 7.23, 5.70 Hz, 1H), 2.682 (m, 1H), 2.719 (m, 1H) 2.814 (ddd, J=12.02, 7.93, 5.96 Hz, 1H) 2.838 (m, 1H) 2.874 (ddd, J=3.44, 9.58, 6.72 Hz, 1H) 3.039 (td, J=11.30, 2.36 Hz, 1H) 3.196 (m, 3H) 3.269 (td, J=8.05, 4.62 Hz, 1H) 3.453 (td, J=8.24, 2.64 Hz, 1H) 3.474 (d, J=2.76 Hz, 1H) 3.743 (td, J=11.20, 5.63 Hz, 1H) 3.797 (m, 3H) 4.087 (td, J=11.18, 5.18 Hz, 1H) 4.226 (d, J=2.88 Hz, 1H) 4.443 (ddd, J=11.82, 10.24, 2.80 Hz, 1H)