Supplementary Material (ESI) for New Journal of Chemistry

S U P P L E M E N T A R Y M A T E R I A L

Sulfoniumcalixpyrrole: The decoration of a calix[4]pyrrole host with positive charges boosts affinity and selectivity of anion binding in DMSO solvent

Martin Valik, Vladimir Král, Eberhardt Herdtweck, and **Franz P. Schmidtchen**

C o n t e n t s

Molecular structure of the thiopyrano calixpyrrole (**6**)

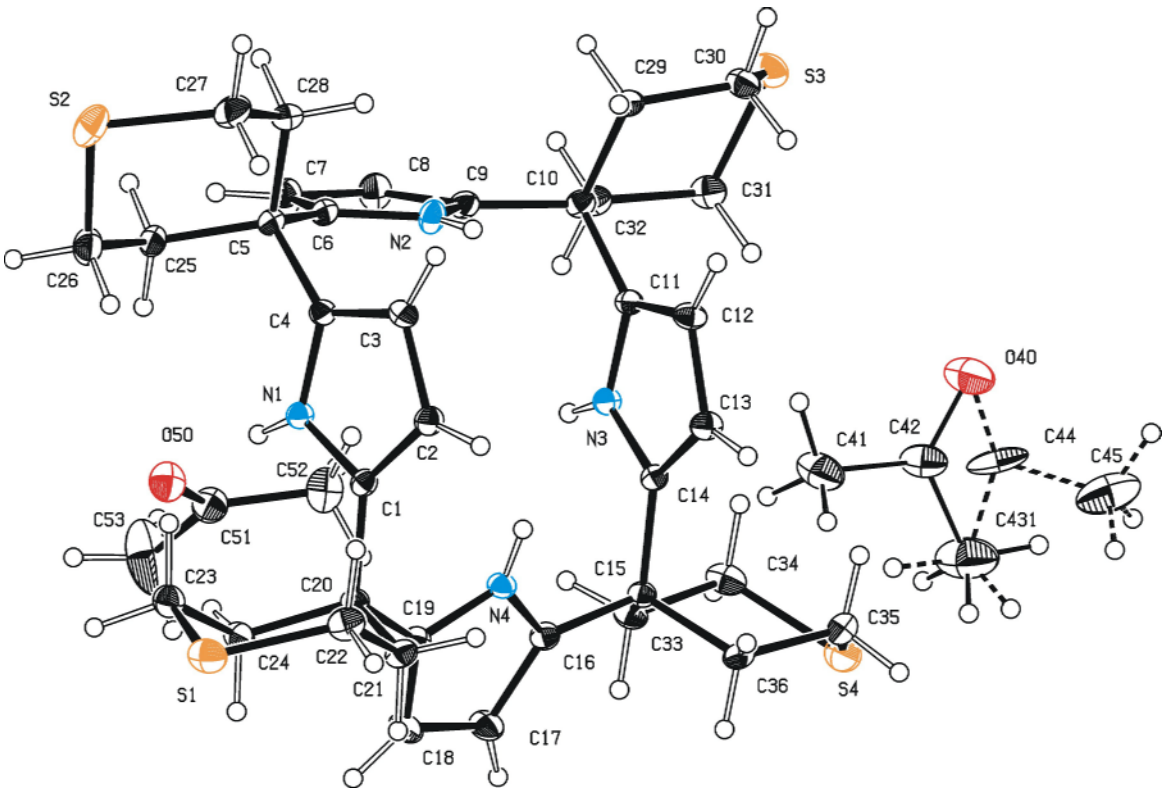


Table S1 - Crystal Data and Details of the Structure Determination for: **Compound 6**

Crystal Data

Formula	C36 H44 N4 S4, 2(C3 H6 O)		
Formula Weight	777.19		
Crystal System	Orthorhombic		
Space group	Pbca		(No. 61)
a, b, c [Angstrom]	16.0948(1)	26.2675(1)	19.2980(1)
V [Ang**3]	8158.62(7)		
Z	8		
D(calc) [g/cm**3]	1.265		
Mu(MoKa) [/mm]	0.274		
F(000)	3328		
Crystal Size [mm]	0.25 x	0.30 x	0.33

Data Collection

Temperature (K)	173		
Radiation [Angstrom]	MoKa		0.71073
Theta Min-Max [Deg]	1.5,		25.4
Dataset	-19: 19 ; -31: 31 ; -23: 23		
Tot., Uniq. Data, R(int)	152651,	7476,	0.044
Observed data [I > 2.0 sigma(I)]	6473		

Refinement

Nref, Npar	7476, 670
R, wR2, S	0.0354, 0.0908, 1.02
w = 1/[\S^2^(FO^2^)+(0.0424P)^2^+5.4301P] WHERE P=(FO^2^+2FC^2^)/3	
Max. and Av. Shift/Error	0.08, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]	-0.45, 0.39

Table S2 - Final Coordinates and Equivalent Isotropic Thermal Parameters of the non-Hydrogen atoms for **Compound 6**

Atom	x	y	z	U(eq) [Ang^2]
S1	0.19061(3)	0.38997(2)	0.07074(2)	0.0354(2)
S2	0.04394(3)	0.56831(2)	0.31661(3)	0.0431(2)
S3	0.21236(3)	0.32264(2)	0.74461(2)	0.0353(2)
S4	0.46284(3)	0.15612(2)	0.51091(3)	0.0404(2)
N1	0.21644(8)	0.41988(5)	0.30271(7)	0.0200(4)
N2	0.19176(9)	0.41791(5)	0.48609(7)	0.0251(4)
N3	0.31952(8)	0.30798(5)	0.50621(7)	0.0206(4)
N4	0.31256(8)	0.30017(5)	0.32311(7)	0.0212(4)
C1	0.20181(9)	0.37438(6)	0.26937(8)	0.0200(4)
C2	0.12495(10)	0.35807(6)	0.29020(8)	0.0243(5)
C3	0.09219(10)	0.39482(6)	0.33676(9)	0.0249(5)
C4	0.14990(10)	0.43279(6)	0.34351(8)	0.0205(4)
C5	0.15313(10)	0.47847(6)	0.39154(8)	0.0231(4)
C6	0.20409(10)	0.46392(6)	0.45412(8)	0.0240(5)
C7	0.26473(12)	0.48841(7)	0.49085(9)	0.0322(6)
C8	0.28905(12)	0.45629(7)	0.54638(9)	0.0313(5)
C9	0.24326(10)	0.41268(6)	0.54233(8)	0.0236(5)
C10	0.23791(10)	0.36530(6)	0.58663(8)	0.0219(5)
C11	0.24589(10)	0.31952(6)	0.53913(7)	0.0198(4)
C12	0.18792(10)	0.28611(6)	0.51499(8)	0.0244(5)
C13	0.22700(10)	0.25305(6)	0.46690(9)	0.0250(5)
C14	0.30896(9)	0.26715(6)	0.46212(8)	0.0196(4)
C15	0.37827(9)	0.24646(6)	0.41711(8)	0.0203(4)
C16	0.38036(9)	0.27485(6)	0.34848(8)	0.0220(5)

Table S2 (cont.) - Final Coordinates and Equivalent Isotropic Thermal Parameters of the non-Hydrogen atoms for **Compound 6**

Atom	x	y	z	U(eq) [Ang^2]
C17	0.44168(11)	0.27954(7)	0.29962(9)	0.0302(5)
C18	0.40950(11)	0.30879(7)	0.24376(9)	0.0305(5)
C19	0.32922(10)	0.32136(6)	0.25961(8)	0.0220(5)
C20	0.26408(9)	0.35123(6)	0.21958(8)	0.0209(4)
C21	0.21856(11)	0.31435(6)	0.16963(9)	0.0261(5)
C22	0.15191(12)	0.33892(7)	0.12469(9)	0.0308(5)
C23	0.24928(12)	0.42552(7)	0.13450(9)	0.0309(5)
C24	0.30824(10)	0.39266(7)	0.17640(9)	0.0247(5)
C25	0.19424(12)	0.52493(6)	0.35680(9)	0.0276(5)
C26	0.14713(13)	0.54584(7)	0.29512(10)	0.0356(6)
C27	0.00608(12)	0.51153(7)	0.35936(11)	0.0372(6)
C28	0.06402(11)	0.49276(7)	0.41598(9)	0.0302(5)
C29	0.15229(11)	0.36596(6)	0.62302(9)	0.0254(5)
C30	0.13758(11)	0.32323(7)	0.67453(9)	0.0294(5)
C31	0.30531(11)	0.32243(7)	0.69199(9)	0.0305(5)
C32	0.30779(11)	0.36655(7)	0.64103(9)	0.0269(5)
C33	0.46288(10)	0.25285(7)	0.45384(9)	0.0253(5)
C34	0.46831(11)	0.22421(8)	0.52236(9)	0.0326(6)
C35	0.36536(12)	0.15473(7)	0.46439(10)	0.0328(6)
C36	0.36383(11)	0.18927(6)	0.40138(9)	0.0259(5)
O40	-0.00829(10)	0.13958(7)	0.45377(8)	0.0556(5)
*C41	0.02548(16)	0.17709(11)	0.34568(13)	0.0527(9)
*C42	0.03594(15)	0.13891(13)	0.40192(14)	0.0416(8)
*C431	0.10101(19)	0.10054(13)	0.39128(15)	0.0792(11)
*C432	0.10101(19)	0.10054(13)	0.39128(15)	0.0792(11)
*C44	0.0361(10)	0.1090(9)	0.4321(12)	0.053(7)
*C45	0.0265(14)	0.0544(8)	0.4467(12)	0.078(9)
O50	0.38098(8)	0.46986(5)	0.30942(7)	0.0374(4)
C51	0.43441(11)	0.45082(7)	0.34502(10)	0.0350(6)
C52	0.41794(14)	0.40695(8)	0.39165(11)	0.0456(7)
C53	0.52168(15)	0.46926(13)	0.33959(19)	0.0933(15)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Starred Atom sites have a S.O.F less than 1.0

Table S3 - Hydrogen Atom Positions and Isotropic Thermal Parameters for **Compound 6**

Atom	x	y	z	U(iso) [Ang^2]
H1	0.2620(13)	0.4356(8)	0.3021(10)	0.033(5)
H2	0.1610(12)	0.3955(8)	0.4730(10)	0.032(5)
H3	0.3657(12)	0.3243(7)	0.5128(9)	0.026(5)
H4	0.2686(12)	0.3030(7)	0.3439(10)	0.029(5)
H21	0.0969(11)	0.3281(7)	0.2739(9)	0.026(4)
H31	0.0419(12)	0.3930(7)	0.3589(10)	0.028(5)
H71	0.2868(12)	0.5206(8)	0.4796(10)	0.037(5)
H81	0.3296(13)	0.4628(8)	0.5801(11)	0.041(6)
H121	0.1318(13)	0.2848(7)	0.5279(10)	0.034(5)
H131	0.2011(11)	0.2259(7)	0.4440(9)	0.029(5)
H171	0.4959(13)	0.2656(8)	0.3026(10)	0.041(5)
H181	0.4372(13)	0.3189(8)	0.2037(11)	0.042(6)
H211	0.2613(12)	0.2985(7)	0.1398(9)	0.030(5)
H212	0.1950(11)	0.2865(7)	0.1960(9)	0.025(4)

Table S3 (cont.) - Hydrogen Atom Positions and Isotropic Thermal Parameters for **Compound 6**

Atom	x	y	z	U(iso) [Ang^2]
H221	0.1061(12)	0.3513(7)	0.1530(9)	0.028(5)
H222	0.1299(13)	0.3153(8)	0.0924(11)	0.044(6)
H231	0.2816(13)	0.4515(8)	0.1064(11)	0.044(6)
H232	0.2088(12)	0.4431(7)	0.1649(10)	0.030(5)
H241	0.3419(11)	0.4140(7)	0.2077(9)	0.027(5)
H242	0.3455(11)	0.3764(6)	0.1447(9)	0.024(4)
H251	0.1981(11)	0.5506(7)	0.3924(9)	0.027(5)
H252	0.2513(12)	0.5159(7)	0.3425(9)	0.030(5)
H261	0.1437(12)	0.5208(8)	0.2590(11)	0.040(5)
H262	0.1771(13)	0.5752(8)	0.2753(10)	0.042(6)
H271	-0.0037(12)	0.4853(8)	0.3241(10)	0.036(5)
H272	-0.0463(14)	0.5213(8)	0.3780(11)	0.045(6)
H281	0.0380(12)	0.4631(8)	0.4398(10)	0.034(5)
H282	0.0700(12)	0.5200(8)	0.4522(10)	0.035(5)
H291	0.1485(11)	0.3983(7)	0.6472(10)	0.029(5)
H292	0.1074(11)	0.3653(7)	0.5887(9)	0.024(4)
H301	0.1399(11)	0.2904(7)	0.6522(10)	0.030(5)
H302	0.0832(13)	0.3269(7)	0.6968(10)	0.036(5)
H311	0.3498(13)	0.3253(8)	0.7242(11)	0.040(5)
H312	0.3092(12)	0.2888(8)	0.6672(10)	0.038(5)
H321	0.3025(11)	0.3976(7)	0.6659(9)	0.026(5)
H322	0.3625(12)	0.3671(7)	0.6167(10)	0.032(5)
H331	0.5073(11)	0.2410(6)	0.4236(9)	0.021(4)
H332	0.4755(11)	0.2893(7)	0.4613(9)	0.028(5)
H341	0.5220(13)	0.2306(7)	0.5437(10)	0.036(5)
H342	0.4238(12)	0.2353(7)	0.5536(10)	0.032(5)
H351	0.3210(12)	0.1639(7)	0.4960(10)	0.035(5)
H352	0.3587(14)	0.1193(9)	0.4510(11)	0.050(6)
H361	0.4054(11)	0.1788(6)	0.3692(9)	0.025(4)
H362	0.3102(12)	0.1850(7)	0.3783(10)	0.030(5)
*H413	0.0772	0.1963	0.3400	0.0790
*H432	0.1556	0.1170	0.3927	0.1190
*H433	0.0932	0.0842	0.3461	0.1190
*H431	0.0977	0.0748	0.4279	0.1190
*H411	-0.0197	0.2005	0.3578	0.0790
*H412	0.0120	0.1596	0.3022	0.0790
*H434	0.0931	0.0684	0.3664	0.1190
*H435	0.1516	0.0985	0.4194	0.1190
*H436	0.1063	0.1284	0.3578	0.1190
*H451	0.0759	0.0419	0.4709	0.1170
*H452	0.0196	0.0358	0.4031	0.1170
*H453	-0.0226	0.0491	0.4759	0.1170
H521	0.3585	0.4056	0.4027	0.0680
H522	0.4499	0.4110	0.4345	0.0680
H523	0.4345	0.3753	0.3685	0.0680
H531	0.5427	0.4775	0.3859	0.1400
H532	0.5234	0.4998	0.3104	0.1400
H533	0.5563	0.4426	0.3188	0.1400

==========

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Starred Atom sites have a S.O.F less than 1.0

Table S4 - (An)isotropic Thermal Parameters for **Compound 6**

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
S1	0.0380(3)	0.0453(3)	0.0229(2)	0.0030(2)	-0.0030(2)	0.0093(2)
S2	0.0528(3)	0.0271(2)	0.0495(3)	0.0048(2)	-0.0087(2)	0.0104(2)
S3	0.0410(3)	0.0452(3)	0.0197(2)	0.0033(2)	-0.0003(2)	0.0052(2)
S4	0.0408(3)	0.0443(3)	0.0360(3)	0.0140(2)	0.0044(2)	0.0180(2)
N1	0.0189(7)	0.0195(7)	0.0215(7)	-0.0018(5)	0.0001(5)	-0.0011(6)
N2	0.0319(8)	0.0186(7)	0.0247(7)	-0.0008(6)	-0.0046(6)	-0.0048(6)
N3	0.0183(7)	0.0206(7)	0.0229(7)	-0.0025(5)	0.0001(5)	-0.0022(6)
N4	0.0174(7)	0.0239(7)	0.0222(7)	0.0003(5)	0.0026(5)	0.0028(6)
C1	0.0212(8)	0.0188(7)	0.0200(8)	0.0002(6)	-0.0021(6)	0.0014(6)
C2	0.0233(8)	0.0219(8)	0.0276(8)	-0.0037(7)	0.0010(7)	-0.0037(7)
C3	0.0214(8)	0.0261(8)	0.0273(8)	0.0002(7)	0.0059(7)	-0.0011(7)
C4	0.0235(8)	0.0201(7)	0.0179(7)	0.0008(6)	0.0012(6)	0.0027(6)
C5	0.0285(8)	0.0184(7)	0.0224(8)	-0.0013(6)	0.0033(7)	0.0022(7)
C6	0.0317(9)	0.0188(8)	0.0214(8)	-0.0022(6)	0.0043(7)	0.0008(7)
C7	0.0449(11)	0.0238(9)	0.0278(9)	-0.0014(7)	-0.0005(8)	-0.0093(8)
C8	0.0386(10)	0.0298(9)	0.0255(9)	-0.0033(7)	-0.0063(8)	-0.0073(8)
C9	0.0290(8)	0.0230(8)	0.0189(8)	-0.0036(6)	-0.0006(7)	0.0019(7)
C10	0.0242(8)	0.0218(8)	0.0196(8)	-0.0022(6)	-0.0026(6)	0.0021(6)
C11	0.0202(7)	0.0219(8)	0.0172(7)	0.0002(6)	0.0005(6)	0.0038(6)
C12	0.0165(8)	0.0308(9)	0.0259(8)	-0.0049(7)	0.0017(6)	-0.0005(7)
C13	0.0212(8)	0.0262(8)	0.0275(8)	-0.0070(7)	0.0000(7)	-0.0034(7)
C14	0.0201(8)	0.0191(7)	0.0195(7)	-0.0014(6)	-0.0008(6)	0.0008(6)
C15	0.0177(7)	0.0224(8)	0.0209(7)	-0.0004(6)	0.0006(6)	0.0015(6)
C16	0.0198(8)	0.0231(8)	0.0231(8)	-0.0002(6)	-0.0015(6)	0.0025(6)
C17	0.0213(8)	0.0380(10)	0.0313(9)	0.0066(8)	0.0044(7)	0.0089(7)
C18	0.0268(9)	0.0400(10)	0.0248(9)	0.0069(8)	0.0061(7)	0.0065(8)
C19	0.0230(8)	0.0227(8)	0.0203(8)	-0.0005(6)	0.0011(6)	0.0013(6)
C20	0.0204(8)	0.0222(8)	0.0202(7)	-0.0004(6)	0.0004(6)	0.0025(6)
C21	0.0303(9)	0.0233(8)	0.0248(8)	-0.0051(7)	-0.0012(7)	0.0031(7)
C22	0.0313(9)	0.0346(10)	0.0264(9)	-0.0054(8)	-0.0062(8)	0.0016(8)
C23	0.0324(9)	0.0313(9)	0.0290(9)	0.0049(8)	0.0022(8)	0.0044(8)
C24	0.0236(8)	0.0284(9)	0.0221(8)	0.0014(7)	0.0020(7)	0.0023(7)
C25	0.0374(10)	0.0191(8)	0.0262(9)	0.0001(7)	0.0024(7)	-0.0008(7)
C26	0.0495(12)	0.0260(9)	0.0312(10)	0.0050(8)	0.0008(9)	-0.0010(9)
C27	0.0337(10)	0.0316(10)	0.0464(11)	-0.0009(9)	0.0030(9)	0.0100(8)
C28	0.0352(10)	0.0257(9)	0.0296(9)	-0.0013(7)	0.0094(8)	0.0064(8)
C29	0.0271(9)	0.0270(9)	0.0220(8)	-0.0026(7)	0.0012(7)	0.0060(7)
C30	0.0291(9)	0.0362(10)	0.0228(8)	0.0016(7)	0.0028(7)	0.0040(8)
C31	0.0313(9)	0.0360(10)	0.0243(9)	-0.0007(8)	-0.0048(7)	0.0052(8)
C32	0.0304(9)	0.0296(9)	0.0207(8)	-0.0063(7)	-0.0042(7)	0.0005(7)
C33	0.0168(8)	0.0340(10)	0.0252(8)	-0.0001(7)	0.0006(7)	0.0022(7)
C34	0.0232(9)	0.0498(11)	0.0247(9)	0.0013(8)	-0.0019(7)	0.0079(8)
C35	0.0396(10)	0.0231(9)	0.0356(10)	0.0009(8)	0.0053(8)	0.0039(8)
C36	0.0293(9)	0.0232(8)	0.0251(8)	-0.0040(7)	0.0031(7)	0.0043(7)
O40	0.0521(9)	0.0739(11)	0.0407(8)	-0.0014(8)	0.0089(7)	0.0138(9)
C41	0.0407(14)	0.0723(19)	0.0451(15)	0.0039(13)	0.0107(11)	0.0069(13)
C42	0.0322(12)	0.0592(18)	0.0335(13)	-0.0090(12)	-0.0020(10)	0.0085(12)
C431	0.0715(18)	0.103(2)	0.0632(17)	-0.0093(16)	0.0038(15)	0.0365(17)
C432	0.0715(18)	0.103(2)	0.0632(17)	-0.0093(16)	0.0038(15)	0.0365(17)
C44	0.034(9)	0.068(14)	0.058(13)	-0.036(11)	-0.010(8)	0.031(9)
C45	0.075(15)	0.075(15)	0.084(16)	-0.042(12)	-0.006(12)	0.017(11)
O50	0.0292(7)	0.0387(7)	0.0442(7)	0.0032(6)	-0.0039(6)	-0.0031(6)
C51	0.0289(9)	0.0353(10)	0.0407(10)	0.0002(8)	0.0002(8)	0.0002(8)
C52	0.0485(12)	0.0403(11)	0.0479(12)	0.0056(9)	-0.0063(10)	-0.0041(10)
C53	0.0350(13)	0.112(3)	0.133(3)	0.066(2)	-0.0216(16)	-0.0191(15)

==========

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for
Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and
h(i) are the Reflection Indices.

Table S5 - Bond Distances (Å) for **Compound 6**

S1	-C22	1.8083(19)	C12	-C13	1.418(2)
S1	-C23	1.8104(19)	C13	-C14	1.373(2)
S2	-C26	1.811(2)	C14	-C15	1.515(2)
S2	-C27	1.810(2)	C15	-C33	1.544(2)
S3	-C30	1.8105(18)	C15	-C36	1.550(2)
S3	-C31	1.8081(18)	C15	-C16	1.520(2)
S4	-C34	1.804(2)	C16	-C17	1.371(2)
S4	-C35	1.808(2)	C17	-C18	1.421(3)
N1	-C1	1.378(2)	C18	-C19	1.368(2)
N1	-C4	1.372(2)	C19	-C20	1.520(2)
N2	-C6	1.371(2)	C20	-C21	1.551(2)
N2	-C9	1.373(2)	C20	-C24	1.544(2)
N3	-C14	1.380(2)	C21	-C22	1.523(3)
N3	-C11	1.378(2)	C23	-C24	1.516(3)
N4	-C16	1.369(2)	C25	-C26	1.514(3)
N4	-C19	1.372(2)	C27	-C28	1.519(3)
C1	-C2	1.369(2)	C29	-C30	1.518(2)
C1	-C20	1.516(2)	C31	-C32	1.520(3)
C2	-C3	1.420(2)	C33	-C34	1.524(3)
C3	-C4	1.369(2)	C35	-C36	1.517(3)
C4	-C5	1.517(2)			
C5	-C28	1.556(2)	O40	-C42	1.228(3)
C5	-C25	1.542(2)	O40	-C44	1.15(2)
C5	-C6	1.509(2)	C41	-C42	1.487(4)
C6	-C7	1.367(2)	C42	-C431	1.468(4)
C7	-C8	1.419(3)	C44	-C432	1.327(19)
C8	-C9	1.364(2)	C44	-C45	1.47(3)
C9	-C10	1.512(2)			
C10	-C29	1.547(2)	O50	-C51	1.209(2)
C10	-C11	1.518(2)	C51	-C52	1.486(3)
C10	-C32	1.539(2)	C51	-C53	1.489(3)
C11	-C12	1.363(2)			
N1	-H1	0.84(2)	C31	-H311	0.95(2)
N2	-H2	0.81(2)	C31	-H312	1.01(2)
N3	-H3	0.867(19)	C32	-H322	0.998(19)
N4	-H4	0.817(19)	C32	-H321	0.950(18)
C2	-H21	0.960(18)	C33	-H331	0.974(17)
C3	-H31	0.917(19)	C33	-H332	0.989(18)
C7	-H71	0.94(2)	C34	-H342	0.981(19)
C8	-H81	0.94(2)	C34	-H341	0.97(2)
C12	-H121	0.94(2)	C35	-H352	0.97(2)
C13	-H131	0.937(18)	C35	-H351	0.969(19)
C17	-H171	0.95(2)	C36	-H362	0.978(19)
C18	-H181	0.93(2)	C36	-H361	0.953(17)
C21	-H211	0.989(19)			
C21	-H212	0.968(18)	C41	-H411	0.98
C22	-H221	0.974(19)	C41	-H412	0.98
C22	-H222	0.95(2)	C41	-H413	0.98
C23	-H231	1.02(2)	C431	-H431	0.98
C23	-H232	0.991(19)	C431	-H432	0.98
C24	-H241	0.986(18)	C431	-H433	0.98
C24	-H242	0.957(17)	C432	-H436	0.98
C25	-H251	0.965(18)	C432	-H434	0.98
C25	-H252	0.988(19)	C432	-H435	0.98
C26	-H261	0.96(2)	C45	-H451	0.98
C26	-H262	0.99(2)	C45	-H452	0.98
C27	-H272	0.95(2)	C45	-H453	0.98
C27	-H271	0.98(2)			
C28	-H281	1.00(2)	C52	-H523	0.98
C28	-H282	1.00(2)	C52	-H522	0.98
C29	-H291	0.971(19)	C52	-H521	0.98
C29	-H292	0.980(18)	C53	-H532	0.98
C30	-H302	0.98(2)	C53	-H531	0.98
C30	-H301	0.965(19)	C53	-H533	0.98

Table S6 - Bond Angles (Degrees) for **Compound 6**

C22	-S1	-C23	99.84(8)	C16	-C15	-C33	109.09(12)
C26	-S2	-C27	98.32(9)	C16	-C15	-C36	107.94(13)
C30	-S3	-C31	97.50(8)	C14	-C15	-C36	110.46(13)
C34	-S4	-C35	97.08(8)	C33	-C15	-C36	109.11(13)
C1	-N1	-C4	110.43(13)	N4	-C16	-C17	106.52(14)
C6	-N2	-C9	110.89(13)	N4	-C16	-C15	122.17(13)
C11	-N3	-C14	110.45(12)	C15	-C16	-C17	131.25(14)
C16	-N4	-C19	111.15(13)	C16	-C17	-C18	107.94(15)
N1	-C1	-C2	106.78(13)	C17	-C18	-C19	107.76(15)
C2	-C1	-C20	131.14(14)	C18	-C19	-C20	131.46(15)
N1	-C1	-C20	122.08(13)	N4	-C19	-C18	106.63(14)
C1	-C2	-C3	107.96(14)	N4	-C19	-C20	121.89(14)
C2	-C3	-C4	107.67(14)	C1	-C20	-C21	109.41(12)
N1	-C4	-C3	107.15(14)	C1	-C20	-C24	111.33(13)
C3	-C4	-C5	131.11(15)	C19	-C20	-C21	108.62(13)
N1	-C4	-C5	121.29(14)	C19	-C20	-C24	108.69(12)
C4	-C5	-C6	107.89(13)	C21	-C20	-C24	108.80(13)
C4	-C5	-C28	110.15(13)	C1	-C20	-C19	109.93(13)
C6	-C5	-C25	108.38(13)	C20	-C21	-C22	114.96(13)
C4	-C5	-C25	112.03(13)	S1	-C22	-C21	113.55(13)
C25	-C5	-C28	109.66(14)	S1	-C23	-C24	113.28(13)
C6	-C5	-C28	108.64(13)	C20	-C24	-C23	113.64(14)
N2	-C6	-C7	106.54(14)	C5	-C25	-C26	114.46(15)
C5	-C6	-C7	133.14(15)	S2	-C26	-C25	113.42(14)
N2	-C6	-C5	120.30(14)	S2	-C27	-C28	112.87(13)
C6	-C7	-C8	107.98(16)	C5	-C28	-C27	115.23(15)
C7	-C8	-C9	107.88(16)	C10	-C29	-C30	115.34(14)
N2	-C9	-C10	119.67(14)	S3	-C30	-C29	113.07(12)
C8	-C9	-C10	133.58(15)	S3	-C31	-C32	112.50(12)
N2	-C9	-C8	106.71(14)	C10	-C32	-C31	113.94(14)
C9	-C10	-C11	107.81(12)	C15	-C33	-C34	113.28(14)
C9	-C10	-C32	109.05(13)	S4	-C34	-C33	112.35(13)
C11	-C10	-C29	111.01(13)	S4	-C35	-C36	113.57(13)
C9	-C10	-C29	107.35(13)	C15	-C36	-C35	114.84(14)
C11	-C10	-C32	111.54(13)				
C29	-C10	-C32	109.95(13)	O40	-C42	-C41	121.3(3)
N3	-C11	-C10	121.70(14)	O40	-C42	-C431	122.5(3)
N3	-C11	-C12	106.82(13)	C41	-C42	-C431	116.2(2)
C10	-C11	-C12	131.21(15)	O40	-C44	-C45	123.0(18)
C11	-C12	-C13	108.32(14)	O40	-C44	-C432	145(2)
C12	-C13	-C14	107.75(14)	C45	-C44	-C432	91.9(16)
N3	-C14	-C15	122.81(13)				
C13	-C14	-C15	130.48(14)	C52	-C51	-C53	117.6(2)
N3	-C14	-C13	106.65(13)	O50	-C51	-C52	122.55(17)
C14	-C15	-C16	109.87(12)	O50	-C51	-C53	119.8(2)
C14	-C15	-C33	110.32(13)				

C4	-N1	-H1	124.5(14)	H281	-C28	-H282	106.0(16)
C1	-N1	-H1	124.6(14)	C10	-C29	-H291	106.5(11)
C6	-N2	-H2	126.1(14)	C10	-C29	-H292	110.5(10)
C9	-N2	-H2	122.9(14)	C30	-C29	-H291	108.8(11)
C14	-N3	-H3	125.5(12)	C30	-C29	-H292	108.3(11)
C11	-N3	-H3	124.1(12)	H291	-C29	-H292	107.1(15)
C19	-N4	-H4	124.8(13)	S3	-C30	-H301	107.5(11)
C16	-N4	-H4	124.0(13)	S3	-C30	-H302	105.5(12)
C1	-C2	-H21	125.8(11)	C29	-C30	-H301	111.2(12)
C3	-C2	-H21	126.1(11)	C29	-C30	-H302	110.7(11)
C2	-C3	-H31	126.0(12)	H301	-C30	-H302	108.6(15)
C4	-C3	-H31	126.4(12)	S3	-C31	-H311	104.8(13)
C6	-C7	-H71	124.9(12)	S3	-C31	-H312	108.7(11)
C8	-C7	-H71	127.1(12)	C32	-C31	-H311	110.0(13)
C7	-C8	-H81	127.4(13)	C32	-C31	-H312	111.1(11)
C9	-C8	-H81	124.7(13)	H311	-C31	-H312	109.5(17)
C11	-C12	-H121	126.3(12)	C10	-C32	-H321	107.3(11)
C13	-C12	-H121	125.4(12)	C10	-C32	-H322	108.9(11)

Table S6 (cont.) - Bond Angles (Degrees) for **Compound 6**

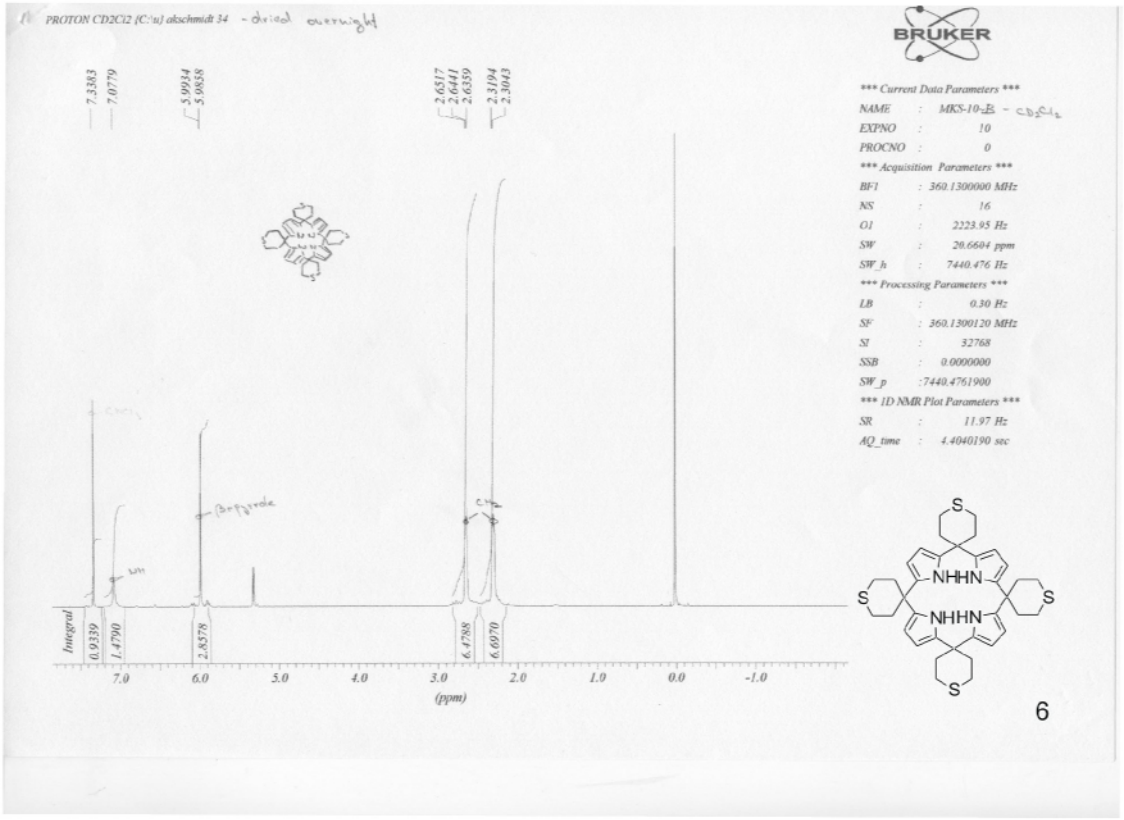
C12	-C13	-H131	125.3(11)	C31	-C32	-H321	109.0(11)
C14	-C13	-H131	126.9(11)	C31	-C32	-H322	109.8(11)
C16	-C17	-H171	125.9(12)	H321	-C32	-H322	107.7(15)
C18	-C17	-H171	126.2(12)	C15	-C33	-H331	109.7(10)
C17	-C18	-H181	127.5(13)	C15	-C33	-H332	110.7(10)
C19	-C18	-H181	124.7(13)	C34	-C33	-H331	108.7(10)
C20	-C21	-H211	107.2(11)	C34	-C33	-H332	109.9(10)
C20	-C21	-H212	109.3(10)	H331	-C33	-H332	104.2(14)
C22	-C21	-H211	109.7(11)	S4	-C34	-H341	105.5(11)
C22	-C21	-H212	110.1(11)	S4	-C34	-H342	109.5(11)
H211	-C21	-H212	105.1(15)	C33	-C34	-H341	109.5(11)
S1	-C22	-H221	109.6(11)	C33	-C34	-H342	110.2(11)
S1	-C22	-H222	103.6(13)	H341	-C34	-H342	109.7(16)
C21	-C22	-H221	110.8(11)	S4	-C35	-H351	108.8(12)
C21	-C22	-H222	111.1(13)	S4	-C35	-H352	104.3(13)
H221	-C22	-H222	107.7(17)	C36	-C35	-H351	110.1(11)
S1	-C23	-H231	104.5(12)	C36	-C35	-H352	111.0(13)
S1	-C23	-H232	107.4(11)	H351	-C35	-H352	108.9(17)
C24	-C23	-H231	110.3(12)	C15	-C36	-H361	107.6(10)
C24	-C23	-H232	111.2(11)	C15	-C36	-H362	109.4(11)
H231	-C23	-H232	109.9(16)	C35	-C36	-H361	109.8(10)
C20	-C24	-H241	108.8(10)	C35	-C36	-H362	108.1(11)
C20	-C24	-H242	108.6(10)	H361	-C36	-H362	106.8(16)
C23	-C24	-H241	110.3(11)				
C23	-C24	-H242	107.8(10)	C42	-C41	-H411	109.43
H241	-C24	-H242	107.5(15)	C42	-C41	-H412	109.48
C5	-C25	-H251	105.7(11)	C42	-C41	-H413	109.44
C5	-C25	-H252	109.3(11)	H411	-C41	-H412	109.49
C26	-C25	-H251	109.8(11)	H411	-C41	-H413	109.50
C26	-C25	-H252	109.4(10)	H412	-C41	-H413	109.48
H251	-C25	-H252	107.9(15)	C44	-C45	-H451	109.48
S2	-C26	-H261	109.7(12)	C44	-C45	-H452	109.52
S2	-C26	-H262	106.4(12)	C44	-C45	-H453	109.48
C25	-C26	-H261	110.5(13)	H451	-C45	-H452	109.55
C25	-C26	-H262	110.1(12)	H451	-C45	-H453	109.44
H261	-C26	-H262	106.4(17)	H452	-C45	-H453	109.36
S2	-C27	-H271	108.5(12)	C42	-C431	-H431	109.53
S2	-C27	-H272	104.4(13)	C42	-C431	-H432	109.45
C28	-C27	-H271	111.7(12)	C42	-C431	-H433	109.49
C28	-C27	-H272	111.1(13)	H431	-C431	-H432	109.47
H271	-C27	-H272	108.0(17)	H431	-C431	-H433	109.43
C5	-C28	-H281	109.8(12)	H432	-C431	-H433	109.47
C5	-C28	-H282	107.1(11)	C44	-C432	-H435	109.54
C27	-C28	-H281	109.1(11)	C44	-C432	-H436	109.55
C27	-C28	-H282	109.2(11)	H434	-C432	-H435	109.41

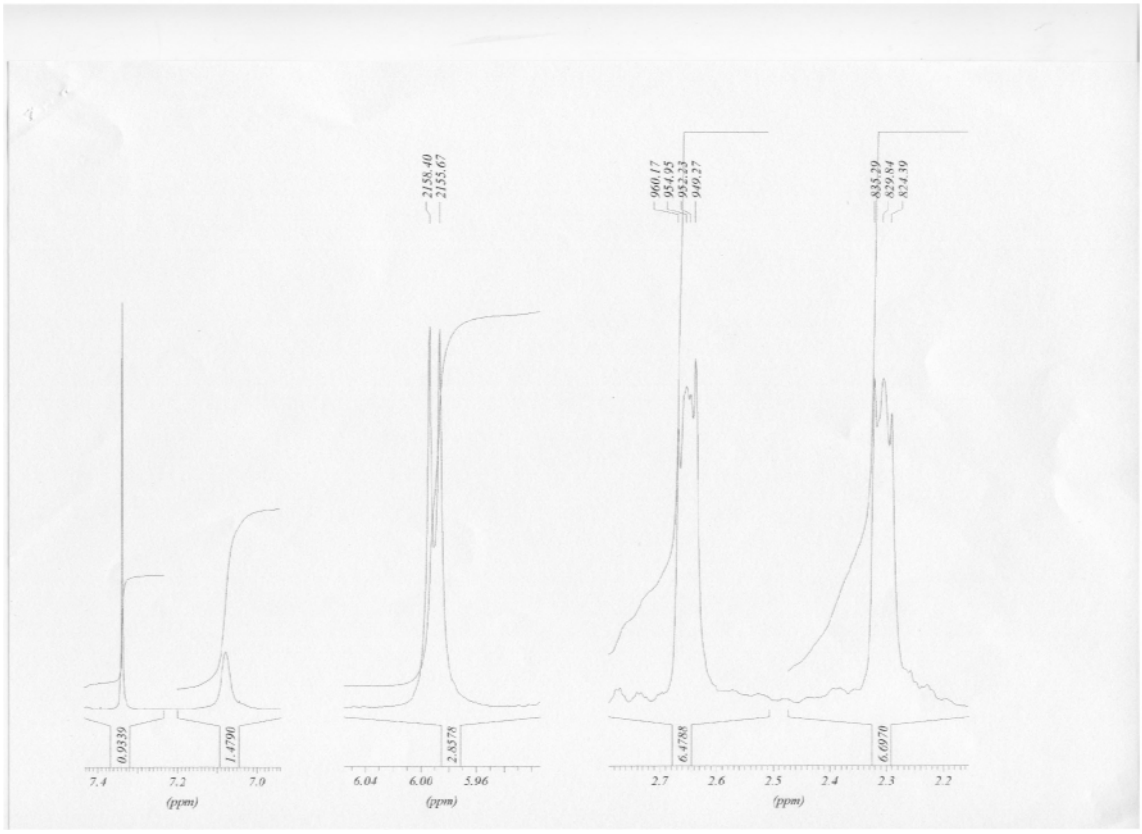
H434	-C432	-H436	109.38
H435	-C432	-H436	109.50

C51	-C52	-H523	109.46
C51	-C52	-H521	109.49
C51	-C52	-H522	109.47
H522	-C52	-H523	109.50
H521	-C52	-H522	109.42
H521	-C52	-H523	109.48
C51	-C53	-H531	109.47
C51	-C53	-H532	109.46
C51	-C53	-H533	109.41
H531	-C53	-H533	109.55
H532	-C53	-H533	109.46
H531	-C53	-H532	109.48

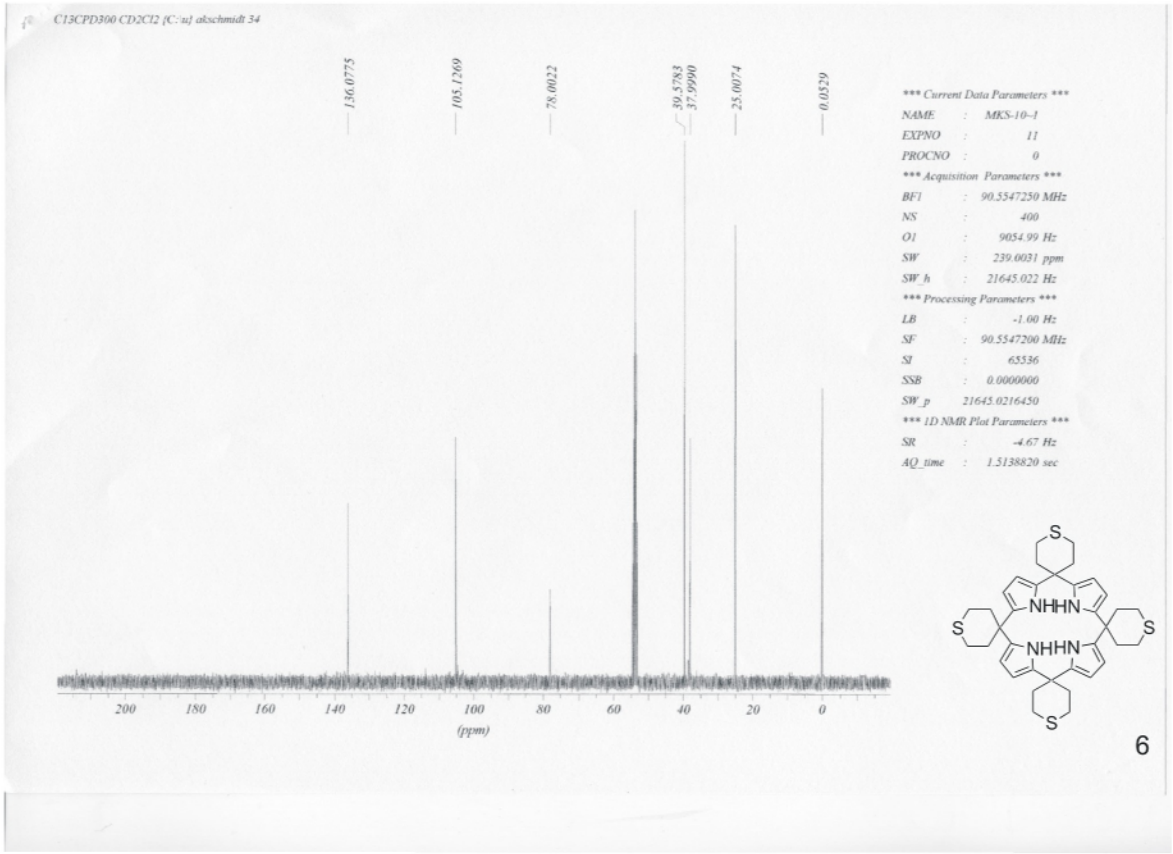
Spectra of the new compounds prepared

1H NMR

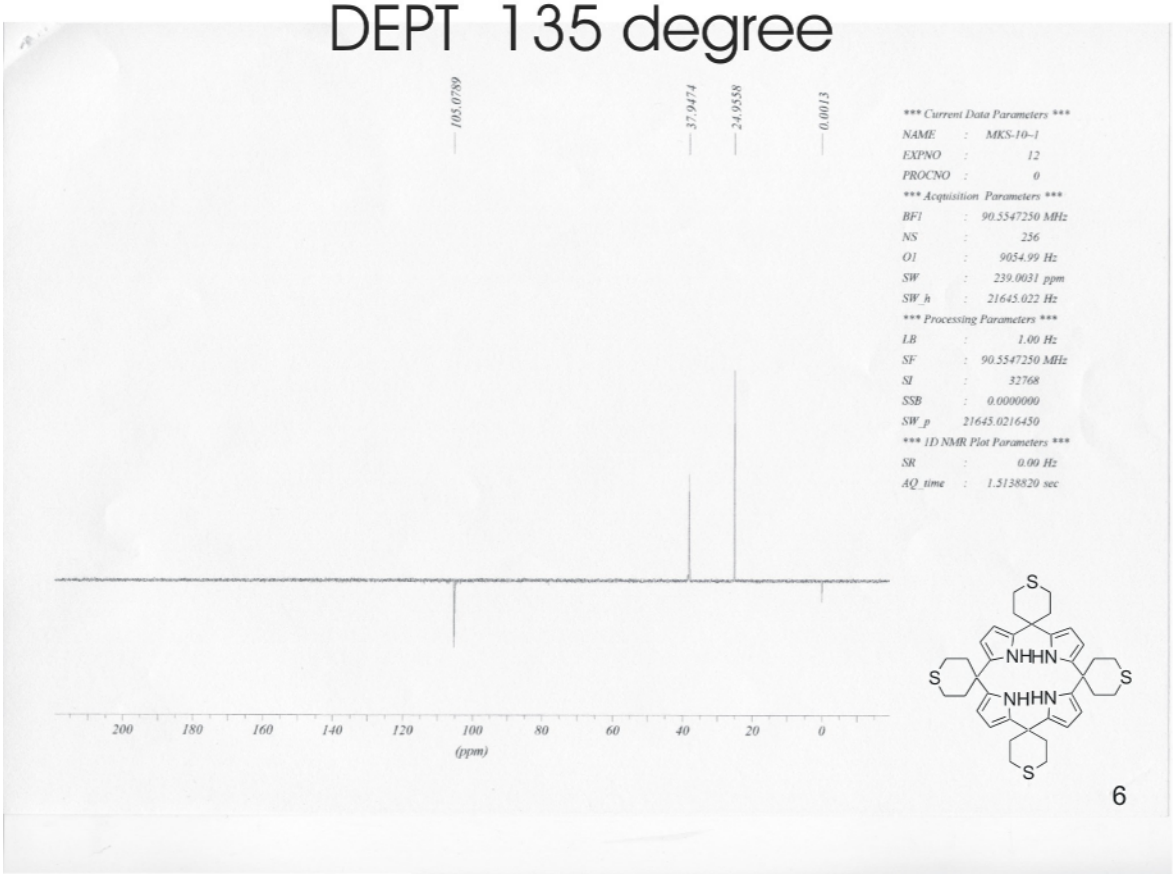




13 carbon spectrum (DMSO)



DEPT 135 degree



Electro spray MS