

Table S1. Bond lengths (Å) of compound **2** using DFT-method from DMOL3 calculations

Bond	Length(Å)	Bond	Length(Å)	Bond	Length(Å)	Bond	Length(Å)
C(30)-H(52)	1.101	C(23)-H(44)	1.094	C(13)-H(40)	1.102	C(6)-H(32)	1.101
C(30)-H(51)	1.101	C(23)-S(24)	1.858	C(13)-H(39)	1.1	C(6)-H(31)	1.095
C(30)-H(50)	1.101	C(21)-C(23)	1.524	C(12)-H(38)	1.09	C(5)-C(15)	1.462
C(29)-H(49)	1.099	C(21)-O(22)	1.232	C(11)-H(37)	1.092	C(4)-O(14)	1.235
C(29)-H(48)	1.1	N(20)-H(43)	1.019	C(11)-C(12)	1.4	C(4)-C(5)	1.465
C(29)-C(30)	1.52	N(20)-C(21)	1.385	C(10)-H(36)	1.092	N(3)-C(7)	1.421
O(28)-C(29)	1.471	C(18)-N(20)	1.398	C(10)-C(11)	1.402	N(3)-C(4)	1.425
C(26)-O(28)	1.372	C(18)-N(19)	1.317	C(9)-H(35)	1.094	N(2)-C(6)	1.479
C(26)-O(27)	1.221	S(17)-C(18)	1.753	C(9)-C(10)	1.401	N(2)-N(3)	1.415
C(25)-H(47)	1.102	C(16)-H(42)	1.085	C(8)-H(34)	1.091	C(1)-C(13)	1.498
C(25)-H(46)	1.1	C(16)-S(17)	1.734	C(8)-C(9)	1.4	C(1)-C(5)	1.386
C(25)-C(26)	1.527	C(15)-N(19)	1.395	C(7)-C(12)	1.407	C(1)-N(2)	1.401
S(24)-C(25)	1.839	C(15)-C(16)	1.386	C(7)-C(8)	1.409		
C(23)-H(45)	1.097	C(13)-H(41)	1.095	C(6)-H(33)	1.1		

Table S2. Bond angles (°) of compound **2** using DFT-method from DMOL3 calculations

Angle	Degree(°)	Angle	Degree(°)	Angle	Degree(°)
H(52)-C(30)-H(51)	108.923	O(22)-C(21)-N(20)	122.438	H(35)-C(9)-C(8)	119.427
H(52)-C(30)-H(50)	107.805	H(43)-N(20)-C(21)	119.288	C(10)-C(9)-C(8)	120.758
H(52)-C(30)-C(29)	111.165	H(43)-N(20)-C(18)	115.479	H(34)-C(8)-C(9)	120.458
H(51)-C(30)-H(50)	108.056	C(21)-N(20)-C(18)	124.872	H(34)-C(8)-C(7)	120.236
H(51)-C(30)-C(29)	111.748	C(18)-N(19)-C(15)	109.545	C(9)-C(8)-C(7)	119.306
H(50)-C(30)-C(29)	109.015	N(20)-C(18)-N(19)	120.556	C(12)-C(7)-C(8)	120.112
H(49)-C(29)-H(48)	107.862	N(20)-C(18)-S(17)	122.657	C(12)-C(7)-N(3)	118.938
H(49)-C(29)-C(30)	111.758	N(19)-C(18)-S(17)	116.787	C(8)-C(7)-N(3)	120.95
H(49)-C(29)-O(28)	108.476	C(18)-S(17)-C(16)	87.529	H(33)-C(6)-H(32)	108.841
H(48)-C(29)-C(30)	112.411	H(42)-C(16)-S(17)	121.483	H(33)-C(6)-H(31)	108.689
H(48)-C(29)-O(28)	108.634	H(42)-C(16)-C(15)	127.006	H(33)-C(6)-N(2)	111.673
C(30)-C(29)-O(28)	107.596	S(17)-C(16)-C(15)	111.484	H(32)-C(6)-H(31)	108.695
C(29)-O(28)-C(26)	115.531	N(19)-C(15)-C(16)	114.553	H(32)-C(6)-N(2)	109.554
O(28)-C(26)-O(27)	125.363	N(19)-C(15)-C(5)	121.262	H(31)-C(6)-N(2)	109.334
O(28)-C(26)-C(25)	112.229	C(16)-C(15)-C(5)	124.185	C(15)-C(5)-C(4)	122.814
O(27)-C(26)-C(25)	122.362	H(41)-C(13)-H(40)	107.979	C(15)-C(5)-C(1)	129.393
H(47)-C(25)-H(46)	107.156	H(41)-C(13)-H(39)	108.897	C(4)-C(5)-C(1)	107.789
H(47)-C(25)-C(26)	109.967	H(41)-C(13)-C(1)	109.577	O(14)-C(4)-C(5)	131.139
H(47)-C(25)-S(24)	110.146	H(40)-C(13)-H(39)	107.43	O(14)-C(4)-N(3)	123.769
H(46)-C(25)-C(26)	107.201	H(40)-C(13)-C(1)	110.343	C(5)-C(4)-N(3)	105.075
H(46)-C(25)-S(24)	105.276	H(39)-C(13)-C(1)	112.489	C(7)-N(3)-C(4)	125.634
C(26)-C(25)-S(24)	116.557	H(38)-C(12)-C(11)	121.133	C(7)-N(3)-N(2)	120.843
C(25)-S(24)-C(23)	100.719	H(38)-C(12)-C(7)	119.054	C(4)-N(3)-N(2)	109.766
H(45)-C(23)-H(44)	110.923	C(11)-C(12)-C(7)	119.803	C(6)-N(2)-N(3)	115.188
H(45)-C(23)-S(24)	108.532	H(37)-C(11)-C(12)	119.13	C(6)-N(2)-C(1)	122.657
H(45)-C(23)-C(21)	111.138	H(37)-C(11)-C(10)	120.549	N(3)-N(2)-C(1)	106.755
H(44)-C(23)-S(24)	108.926	C(12)-C(11)-C(10)	120.306	C(13)-C(1)-C(5)	128.748
H(44)-C(23)-C(21)	108.237	H(36)-C(10)-C(11)	120.029	C(13)-C(1)-N(2)	120.862
S(24)-C(23)-C(21)	109.043	H(36)-C(10)-C(9)	120.345	C(5)-C(1)-N(2)	110.352
C(23)-C(21)-O(22)	122.534	C(11)-C(10)-C(9)	119.622		
C(23)-C(21)-N(20)	114.959	H(35)-C(9)-C(10)	119.788		

Table S3. Bond lengths (Å) of compound **4** using DFT-method from DMOL3 calculations

Bond	Length(Å)	Bond	Length(Å)	Bond	Length(Å)	Bond	Length(Å)
C(34)-H(57)	1.09	N(26)-C(27)	1.352	C(16)-S(17)	1.732	C(7)-C(12)	1.408
N(33)-C(34)	1.192	C(25)-C(30)	1.422	C(15)-N(19)	1.398	C(7)-C(8)	1.406
C(32)-H(56)	1.102	C(25)-N(26)	1.342	C(15)-C(16)	1.384	C(6)-H(37)	1.101
C(32)-H(55)	1.1	S(24)-C(25)	1.799	C(13)-H(45)	1.094	C(6)-H(36)	1.097
C(32)-H(54)	1.096	C(23)-H(49)	1.1	C(13)-H(44)	1.105	C(6)-H(35)	1.094
C(31)-H(53)	1.102	C(23)-H(48)	1.095	C(13)-H(43)	1.1	C(5)-C(15)	1.464
C(31)-H(52)	1.097	C(23)-S(24)	1.865	C(12)-H(42)	1.09	C(4)-O(14)	1.237
C(31)-H(51)	1.098	C(21)-C(23)	1.536	C(11)-H(41)	1.093	C(4)-C(5)	1.47
C(30)-N(33)	1.384	C(21)-O(22)	1.234	C(11)-C(12)	1.398	N(3)-C(7)	1.424
C(29)-C(32)	1.513	N(20)-H(47)	1.016	C(10)-H(40)	1.092	N(3)-C(4)	1.426
C(29)-C(30)	1.417	N(20)-C(21)	1.386	C(10)-C(11)	1.401	N(2)-C(6)	1.479
C(28)-H(50)	1.094	C(18)-N(20)	1.401	C(9)-H(39)	1.094	N(2)-N(3)	1.417
C(28)-C(29)	1.4	C(18)-N(19)	1.316	C(9)-C(10)	1.401	C(1)-C(13)	1.5
C(27)-C(31)	1.51	S(17)-C(18)	1.753	C(8)-H(38)	1.092	C(1)-C(5)	1.381
C(27)-C(28)	1.403	C(16)-H(46)	1.086	C(8)-C(9)	1.402	C(1)-N(2)	1.402

Table S4. Bond angles (°) of compound **4** using DFT-method from DMOL3 calculations

Angle	Degree(°)	Angle	Degree(°)	Angle	Degree(°)
H(57)-C(34)-N(33)	180	H(49)-C(23)-C(21)	112.968	H(40)-C(10)-C(11)	120.387
C(34)-N(33)-C(30)	175.55	H(48)-C(23)-S(24)	111.115	H(40)-C(10)-C(9)	120.291
H(56)-C(32)-H(55)	107.456	H(48)-C(23)-C(21)	106.615	C(11)-C(10)-C(9)	119.322
H(56)-C(32)-H(54)	107.641	S(24)-C(23)-C(21)	105.917	H(39)-C(9)-C(10)	120.086
H(56)-C(32)-C(29)	110.309	C(23)-C(21)-O(22)	121.741	H(39)-C(9)-C(8)	119.344
H(55)-C(32)-H(54)	109.1	C(23)-C(21)-N(20)	116.173	C(10)-C(9)-C(8)	120.526
H(55)-C(32)-C(29)	110.396	O(22)-C(21)-N(20)	122.081	H(38)-C(8)-C(9)	120.471
H(54)-C(32)-C(29)	111.802	H(47)-N(20)-C(21)	120.465	H(38)-C(8)-C(7)	119.701
H(53)-C(31)-H(52)	107.443	H(47)-N(20)-C(18)	114.892	C(9)-C(8)-C(7)	119.827
H(53)-C(31)-H(51)	107.837	C(21)-N(20)-C(18)	124.642	C(12)-C(7)-C(8)	119.747
H(53)-C(31)-C(27)	109.873	C(18)-N(19)-C(15)	110.035	C(12)-C(7)-N(3)	118.4
H(52)-C(31)-H(51)	109.616	N(20)-C(18)-N(19)	121.417	C(8)-C(7)-N(3)	121.853
H(52)-C(31)-C(27)	110.226	N(20)-C(18)-S(17)	122.33	H(37)-C(6)-H(36)	109.267
H(51)-C(31)-C(27)	111.723	N(19)-C(18)-S(17)	116.208	H(37)-C(6)-H(35)	110.101
N(33)-C(30)-C(29)	118.988	C(18)-S(17)-C(16)	87.976	H(37)-C(6)-N(2)	111.939
N(33)-C(30)-C(25)	121.804	H(46)-C(16)-S(17)	121.689	H(36)-C(6)-H(35)	108.255
C(29)-C(30)-C(25)	119.182	H(46)-C(16)-C(15)	126.934	H(36)-C(6)-N(2)	108.818
C(32)-C(29)-C(30)	121.884	S(17)-C(16)-C(15)	111.374	H(35)-C(6)-N(2)	108.38
C(32)-C(29)-C(28)	120.918	N(19)-C(15)-C(16)	114.406	C(15)-C(5)-C(4)	122.136
C(30)-C(29)-C(28)	117.155	N(19)-C(15)-C(5)	121.553	C(15)-C(5)-C(1)	130.055
H(50)-C(28)-C(29)	119.424	C(16)-C(15)-C(5)	124.04	C(4)-C(5)-C(1)	107.778
H(50)-C(28)-C(27)	120.046	H(45)-C(13)-H(44)	107.27	O(14)-C(4)-C(5)	131.47
C(29)-C(28)-C(27)	120.522	H(45)-C(13)-H(43)	109.617	O(14)-C(4)-N(3)	123.712
C(31)-C(27)-C(28)	121.709	H(45)-C(13)-C(1)	109.64	C(5)-C(4)-N(3)	104.795
C(31)-C(27)-N(26)	116.607	H(44)-C(13)-H(43)	107.794	C(7)-N(3)-C(4)	125.075
C(28)-C(27)-N(26)	121.675	H(44)-C(13)-C(1)	111.053	C(7)-N(3)-N(2)	120.197
C(27)-N(26)-C(25)	119.47	H(43)-C(13)-C(1)	111.361	C(4)-N(3)-N(2)	109.827
C(30)-C(25)-N(26)	121.918	H(42)-C(12)-C(11)	120.86	C(6)-N(2)-N(3)	114.102
C(30)-C(25)-S(24)	126.604	H(42)-C(12)-C(7)	119.371	C(6)-N(2)-C(1)	120.072
N(26)-C(25)-S(24)	111.084	C(11)-C(12)-C(7)	119.766	N(3)-N(2)-C(1)	106.408
C(25)-S(24)-C(23)	108.016	H(41)-C(11)-C(12)	119.104	C(13)-C(1)-C(5)	130.518
H(49)-C(23)-H(48)	110.809	H(41)-C(11)-C(10)	120.12	C(13)-C(1)-N(2)	118.821
H(49)-C(23)-S(24)	109.312	C(12)-C(11)-C(10)	120.776	C(5)-C(1)-N(2)	110.639

Table S5. Bond lengths (Å) of compound **5** using DFT-method from DMOL3 calculations

Bond	Length(Å)	Bond	Length(Å)	Bond	Length(Å)	Bond	Length(Å)
N(34)-H(56)	1.012	C(27)-C(28)	1.415	C(16)-S(17)	1.733	C(7)-C(12)	1.41
N(34)-H(55)	1.023	N(26)-C(27)	1.348	C(15)-N(19)	1.391	C(7)-C(8)	1.408
C(33)-N(34)	1.381	C(25)-C(30)	1.425	C(15)-C(16)	1.385	C(6)-H(37)	1.099
C(32)-H(54)	1.1	C(25)-N(26)	1.338	C(13)-H(45)	1.094	C(6)-H(36)	1.1
C(32)-H(53)	1.098	S(24)-C(25)	1.757	C(13)-H(44)	1.103	C(6)-H(35)	1.096
C(32)-H(52)	1.104	C(23)-C(33)	1.402	C(13)-H(43)	1.1	C(5)-C(15)	1.46
C(31)-H(51)	1.103	C(23)-S(24)	1.775	C(12)-H(42)	1.086	C(4)-O(14)	1.235
C(31)-H(50)	1.097	C(21)-C(23)	1.467	C(11)-H(41)	1.092	C(4)-C(5)	1.461
C(31)-H(49)	1.098	C(21)-O(22)	1.244	C(11)-C(12)	1.398	N(3)-C(7)	1.429
C(30)-C(33)	1.454	N(20)-H(47)	1.015	C(10)-H(40)	1.092	N(3)-C(4)	1.44
C(29)-C(32)	1.512	N(20)-C(21)	1.404	C(10)-C(11)	1.402	N(2)-C(6)	1.478
C(29)-C(30)	1.423	C(18)-N(20)	1.394	C(9)-H(39)	1.092	N(2)-N(3)	1.418
C(28)-H(48)	1.092	C(18)-N(19)	1.303	C(9)-C(10)	1.403	C(1)-C(13)	1.501
C(28)-C(29)	1.399	S(17)-C(18)	1.777	C(8)-H(38)	1.09	C(1)-C(5)	1.386
C(27)-C(31)	1.509	C(16)-H(46)	1.084	C(8)-C(9)	1.4	C(1)-N(2)	1.39

Table S6. Bond angles (°) of compound **5** using DFT-method from DMOL3 calculations

Angle	Degree(°)	Angle	Degree(°)	Angle	Degree(°)
H(56)-N(34)-H(55)	115.923	C(25)-S(24)-C(23)	90.84	H(40)-C(10)-C(9)	120.327
H(56)-N(34)-C(33)	116.952	C(33)-C(23)-S(24)	112.483	C(11)-C(10)-C(9)	119.214
H(55)-N(34)-C(33)	112.191	C(33)-C(23)-C(21)	124.53	H(39)-C(9)-C(10)	120.123
N(34)-C(33)-C(30)	125.049	S(24)-C(23)-C(21)	122.84	H(39)-C(9)-C(8)	119.361
N(34)-C(33)-C(23)	122.449	C(23)-C(21)-O(22)	123.596	C(10)-C(9)-C(8)	120.486
C(30)-C(33)-C(23)	112.437	C(23)-C(21)-N(20)	114.345	H(38)-C(8)-C(9)	119.888
H(54)-C(32)-H(53)	108.165	O(22)-C(21)-N(20)	122.053	H(38)-C(8)-C(7)	119.965
H(54)-C(32)-H(52)	107.892	H(47)-N(20)-C(21)	116.136	C(9)-C(8)-C(7)	120.117
H(54)-C(32)-C(29)	111.566	H(47)-N(20)-C(18)	115.012	C(12)-C(7)-C(8)	119.505
H(53)-C(32)-H(52)	107.017	C(21)-N(20)-C(18)	128.402	C(12)-C(7)-N(3)	118.493
H(53)-C(32)-C(29)	110.873	C(18)-N(19)-C(15)	110.577	C(8)-C(7)-N(3)	121.992
H(52)-C(32)-C(29)	111.146	N(20)-C(18)-N(19)	126.952	H(37)-C(6)-H(36)	109.056
H(51)-C(31)-H(50)	107.275	N(20)-C(18)-S(17)	117.64	H(37)-C(6)-H(35)	108.52
H(51)-C(31)-H(49)	107.79	N(19)-C(18)-S(17)	115.401	H(37)-C(6)-N(2)	110.872
H(51)-C(31)-C(27)	110.021	C(18)-S(17)-C(16)	88.061	H(36)-C(6)-H(35)	108.657
H(50)-C(31)-H(49)	109.389	H(46)-C(16)-S(17)	121.547	H(36)-C(6)-N(2)	110.369
H(50)-C(31)-C(27)	110.059	H(46)-C(16)-C(15)	127.693	H(35)-C(6)-N(2)	109.316
H(49)-C(31)-C(27)	112.16	S(17)-C(16)-C(15)	110.708	C(15)-C(5)-C(4)	122.03
C(33)-C(30)-C(29)	132.408	N(19)-C(15)-C(16)	115.208	C(15)-C(5)-C(1)	129.421
C(33)-C(30)-C(25)	111.659	N(19)-C(15)-C(5)	120.531	C(4)-C(5)-C(1)	108.146
C(29)-C(30)-C(25)	115.924	C(16)-C(15)-C(5)	124.202	O(14)-C(4)-C(5)	131.222
C(32)-C(29)-C(30)	124.098	H(45)-C(13)-H(44)	106.984	O(14)-C(4)-N(3)	123.775
C(32)-C(29)-C(28)	118.992	H(45)-C(13)-H(43)	109.588	C(5)-C(4)-N(3)	105.002
C(30)-C(29)-C(28)	116.902	H(45)-C(13)-C(1)	110.569	C(7)-N(3)-C(4)	122.424
H(48)-C(28)-C(29)	119.131	H(44)-C(13)-H(43)	107.054	C(7)-N(3)-N(2)	118.253
H(48)-C(28)-C(27)	118.893	H(44)-C(13)-C(1)	110.022	C(4)-N(3)-N(2)	108.569
C(29)-C(28)-C(27)	121.974	H(43)-C(13)-C(1)	112.42	C(6)-N(2)-N(3)	116.792
C(31)-C(27)-C(28)	121.38	H(42)-C(12)-C(11)	120.912	C(6)-N(2)-C(1)	122.943
C(31)-C(27)-N(26)	116.74	H(42)-C(12)-C(7)	119.368	N(3)-N(2)-C(1)	107.672
C(28)-C(27)-N(26)	121.82	C(11)-C(12)-C(7)	119.718	C(13)-C(1)-C(5)	130.012
C(27)-N(26)-C(25)	115.956	H(41)-C(11)-C(12)	118.929	C(13)-C(1)-N(2)	119.859
C(30)-C(25)-N(26)	127.364	H(41)-C(11)-C(10)	120.12	C(5)-C(1)-N(2)	110.109
C(30)-C(25)-S(24)	112.565	C(12)-C(11)-C(10)	120.876		
N(26)-C(25)-S(24)	120.069	H(40)-C(10)-C(11)	120.453		

Table S7. Bond lengths (Å) of compound **6** using DFT-method from DMOL3 calculations

Bond	Length(Å)	Bond	Length(Å)	Bond	Length(Å)	Bond	Length(Å)
N(36)-H(56)	1.02	C(27)-C(28)	1.413	C(15)-N(19)	1.379	C(7)-C(8)	1.402
N(36)-H(55)	1.02	N(26)-C(27)	1.418	C(15)-C(16)	1.407	C(6)-H(39)	1.099
S(33)-N(36)	1.701	N(25)-N(26)	1.288	C(13)-H(47)	1.097	C(6)-H(38)	1.098
S(33)-O(35)	1.473	C(23)-H(50)	1.097	C(13)-H(46)	1.101	C(6)-H(37)	1.098
S(33)-O(34)	1.472	C(23)-H(49)	1.097	C(13)-H(45)	1.099	C(5)-C(15)	1.457
C(32)-H(54)	1.089	C(23)-Cl(24)	1.789	C(12)-H(44)	1.09	C(4)-O(14)	1.233
C(31)-H(53)	1.09	C(21)-C(23)	1.539	C(11)-H(43)	1.092	C(4)-C(5)	1.469
C(31)-C(32)	1.398	C(21)-O(22)	1.227	C(11)-C(12)	1.399	N(3)-C(7)	1.417
C(30)-S(33)	1.8	N(20)-H(48)	1.018	C(10)-H(42)	1.09	N(3)-C(4)	1.428
C(30)-C(31)	1.4	N(20)-C(21)	1.393	C(10)-C(11)	1.402	N(2)-C(6)	1.472
C(29)-H(52)	1.089	C(18)-N(20)	1.394	C(9)-H(41)	1.093	N(2)-N(3)	1.411
C(29)-C(30)	1.406	C(18)-N(19)	1.328	C(9)-C(10)	1.399	C(1)-C(13)	1.499
C(28)-H(51)	1.091	S(17)-C(18)	1.743	C(8)-H(40)	1.093	C(1)-C(5)	1.389
C(28)-C(29)	1.394	C(16)-N(25)	1.358	C(8)-C(9)	1.399	C(1)-N(2)	1.381
C(27)-C(32)	1.409	C(16)-S(17)	1.79	C(7)-C(12)	1.404		

Table S8. Bond angles (°) of compound **6** using DFT-method from DMOL3 calculations

Angle	Degree(°)	Angle	Degree(°)	Angle	Degree(°)
H(56)-N(36)-H(55)	109.511	H(49)-C(23)-C(21)	112.493	C(11)-C(10)-C(9)	120.086
H(56)-N(36)-S(33)	106.57	Cl(24)-C(23)-C(21)	112.184	H(41)-C(9)-C(10)	119.904
H(55)-N(36)-S(33)	105.55	C(23)-C(21)-O(22)	124.12	H(41)-C(9)-C(8)	119.618
N(36)-S(33)-O(35)	108.608	C(23)-C(21)-N(20)	113.596	C(10)-C(9)-C(8)	120.478
N(36)-S(33)-O(34)	106.581	O(22)-C(21)-N(20)	122.172	H(40)-C(8)-C(9)	121.314
N(36)-S(33)-C(30)	101.974	H(48)-N(20)-C(21)	120.232	H(40)-C(8)-C(7)	119.466
O(35)-S(33)-O(34)	122.138	H(48)-N(20)-C(18)	113.97	C(9)-C(8)-C(7)	119.218
O(35)-S(33)-C(30)	107.573	C(21)-N(20)-C(18)	125.641	C(12)-C(7)-C(8)	120.576
O(34)-S(33)-C(30)	108.156	C(18)-N(19)-C(15)	110.236	C(12)-C(7)-N(3)	118.089
H(54)-C(32)-C(31)	120.756	N(20)-C(18)-N(19)	118.879	C(8)-C(7)-N(3)	121.332
H(54)-C(32)-C(27)	118.919	N(20)-C(18)-S(17)	122.968	H(39)-C(6)-H(38)	108.496
C(31)-C(32)-C(27)	120.316	N(19)-C(18)-S(17)	118.152	H(39)-C(6)-H(37)	109.334
H(53)-C(31)-C(32)	120.447	C(18)-S(17)-C(16)	86.433	H(39)-C(6)-N(2)	111.162
H(53)-C(31)-C(30)	120.099	N(25)-C(16)-S(17)	124.899	H(38)-C(6)-H(37)	108.509
C(32)-C(31)-C(30)	119.416	N(25)-C(16)-C(15)	124.338	H(38)-C(6)-N(2)	109.144
S(33)-C(30)-C(31)	122.108	S(17)-C(16)-C(15)	110.745	H(37)-C(6)-N(2)	110.137
S(33)-C(30)-C(29)	116.841	N(19)-C(15)-C(16)	114.387	C(15)-C(5)-C(4)	125.028
C(31)-C(30)-C(29)	120.989	N(19)-C(15)-C(5)	121.443	C(15)-C(5)-C(1)	126.688
H(52)-C(29)-C(30)	120.179	C(16)-C(15)-C(5)	124.111	C(4)-C(5)-C(1)	108.245
H(52)-C(29)-C(28)	120.406	H(47)-C(13)-H(46)	107.081	O(14)-C(4)-C(5)	133.277
C(30)-C(29)-C(28)	119.41	H(47)-C(13)-H(45)	108.96	O(14)-C(4)-N(3)	122.88
H(51)-C(28)-C(29)	120.952	H(47)-C(13)-C(1)	109.855	C(5)-C(4)-N(3)	103.828
H(51)-C(28)-C(27)	118.723	H(46)-C(13)-H(45)	107.894	C(7)-N(3)-C(4)	125.272
C(29)-C(28)-C(27)	120.288	H(46)-C(13)-C(1)	110.29	C(7)-N(3)-N(2)	122.359
C(32)-C(27)-C(28)	119.54	H(45)-C(13)-C(1)	112.588	C(4)-N(3)-N(2)	110.285
C(32)-C(27)-N(26)	116.843	H(44)-C(12)-C(11)	121.075	C(6)-N(2)-N(3)	118.491
C(28)-C(27)-N(26)	123.587	H(44)-C(12)-C(7)	119.174	C(6)-N(2)-C(1)	124.919
C(27)-N(26)-N(25)	112.332	C(11)-C(12)-C(7)	119.75	N(3)-N(2)-C(1)	107.217
N(26)-N(25)-C(16)	116.245	H(43)-C(11)-C(12)	119.933	C(13)-C(1)-C(5)	129.04
H(50)-C(23)-H(49)	108.991	H(43)-C(11)-C(10)	120.197	C(13)-C(1)-N(2)	120.691
H(50)-C(23)-Cl(24)	107.172	C(12)-C(11)-C(10)	119.87	C(5)-C(1)-N(2)	110.268
H(50)-C(23)-C(21)	108.171	H(42)-C(10)-C(11)	120.139		
H(49)-C(23)-Cl(24)	107.663	H(42)-C(10)-C(9)	119.757		

Table S9. Bond lengths (Å) of compound **7a** using DFT-method from DMOL3 calculations

Bond	Length(Å)	Bond	Length(Å)	Bond	Length(Å)	Bond	Length(Å)
C(45)-H(69)	1.089	S(32)-O(33)	1.474	N(20)-H(57)	1.019	C(8)-H(49)	1.093
C(44)-H(68)	1.089	C(31)-H(63)	1.092	N(20)-C(21)	1.394	C(8)-C(9)	1.399
C(44)-C(45)	1.396	C(30)-H(62)	1.09	C(18)-N(20)	1.398	C(7)-C(12)	1.406
C(43)-H(67)	1.094	C(30)-C(31)	1.4	C(18)-N(19)	1.327	C(7)-C(8)	1.408
C(43)-C(44)	1.408	C(29)-S(32)	1.799	S(17)-C(18)	1.746	C(6)-H(48)	1.099
C(42)-H(66)	1.089	C(29)-C(30)	1.404	C(16)-N(24)	1.359	C(6)-H(47)	1.096
C(42)-C(43)	1.398	C(28)-H(61)	1.09	C(16)-S(17)	1.784	C(6)-H(46)	1.096
C(40)-C(45)	1.404	C(28)-C(29)	1.407	C(15)-N(19)	1.381	C(5)-C(15)	1.461
C(40)-N(41)	1.392	C(27)-H(60)	1.091	C(15)-C(16)	1.409	C(4)-O(14)	1.235
C(39)-C(42)	1.4	C(27)-C(28)	1.393	C(13)-H(56)	1.097	C(4)-C(5)	1.47
C(39)-C(40)	1.422	C(26)-C(31)	1.409	C(13)-H(55)	1.102	N(3)-C(7)	1.418
S(38)-C(39)	1.758	C(26)-C(27)	1.421	C(13)-H(54)	1.099	N(3)-C(4)	1.426
C(37)-N(41)	1.31	N(25)-C(26)	1.415	C(12)-H(53)	1.09	N(2)-C(6)	1.468
C(37)-S(38)	1.786	N(24)-N(25)	1.289	C(11)-H(52)	1.093	N(2)-N(3)	1.408
S(36)-C(37)	1.765	C(23)-H(59)	1.099	C(11)-C(12)	1.397	C(1)-C(13)	1.5
N(35)-H(65)	1.018	C(23)-H(58)	1.098	C(10)-H(51)	1.093	C(1)-C(5)	1.393
N(35)-H(64)	1.017	C(23)-S(36)	1.859	C(10)-C(11)	1.405	C(1)-N(2)	1.377
S(32)-N(35)	1.684	C(21)-C(23)	1.524	C(9)-H(50)	1.092		
S(32)-O(34)	1.473	C(21)-O(22)	1.234	C(9)-C(10)	1.403		

Table S10. Bond angles (°) of compound **7a** using DFT-method from DMOL3 calculations

Angle	Degree(°)	Angle	Degree(°)	Angle	Degree(°)
H(69)-C(45)-C(44)	120.937	C(30)-C(29)-C(28)	120.951	H(53)-C(12)-C(11)	121.22
H(69)-C(45)-C(40)	119.541	H(61)-C(28)-C(29)	119.847	H(53)-C(12)-C(7)	119.066
C(44)-C(45)-C(40)	119.488	H(61)-C(28)-C(27)	120.31	C(11)-C(12)-C(7)	119.714
H(68)-C(44)-C(45)	119.437	C(29)-C(28)-C(27)	119.83	H(52)-C(11)-C(12)	119.604
H(68)-C(44)-C(43)	119.311	H(60)-C(27)-C(28)	121.417	H(52)-C(11)-C(10)	120.269
C(45)-C(44)-C(43)	121.252	H(60)-C(27)-C(26)	118.802	C(12)-C(11)-C(10)	120.125
H(67)-C(43)-C(44)	119.958	C(28)-C(27)-C(26)	119.757	H(51)-C(10)-C(11)	119.658
H(67)-C(43)-C(42)	119.828	C(31)-C(26)-C(27)	119.784	H(51)-C(10)-C(9)	120.435
C(44)-C(43)-C(42)	120.215	C(31)-C(26)-N(25)	116.623	C(11)-C(10)-C(9)	119.907
H(66)-C(42)-C(43)	121.368	C(27)-C(26)-N(25)	123.515	H(50)-C(9)-C(10)	119.733
H(66)-C(42)-C(39)	120.181	C(26)-N(25)-N(24)	112.356	H(50)-C(9)-C(8)	119.797
C(43)-C(42)-C(39)	118.449	N(25)-N(24)-C(16)	115.471	C(10)-C(9)-C(8)	120.467
C(40)-N(41)-C(37)	110.125	H(59)-C(23)-H(58)	108.984	H(49)-C(8)-C(9)	121.081
C(45)-C(40)-N(41)	125.738	H(59)-C(23)-S(36)	108.914	H(49)-C(8)-C(7)	119.6
C(45)-C(40)-C(39)	118.632	H(59)-C(23)-C(21)	112.633	C(9)-C(8)-C(7)	119.312
N(41)-C(40)-C(39)	115.623	H(58)-C(23)-S(36)	108.051	C(12)-C(7)-C(8)	120.464
C(42)-C(39)-C(40)	121.935	H(58)-C(23)-C(21)	107.439	C(12)-C(7)-N(3)	118.06
C(42)-C(39)-S(38)	128.406	S(36)-C(23)-C(21)	110.699	C(8)-C(7)-N(3)	121.475
C(40)-C(39)-S(38)	109.655	C(23)-C(21)-O(22)	121.718	H(48)-C(6)-H(47)	108.285
C(39)-S(38)-C(37)	87.866	C(23)-C(21)-N(20)	116.189	H(48)-C(6)-H(46)	109.545
N(41)-C(37)-S(38)	116.619	O(22)-C(21)-N(20)	122.084	H(48)-C(6)-N(2)	111.64
N(41)-C(37)-S(36)	125.538	H(57)-N(20)-C(21)	120.243	H(47)-C(6)-H(46)	107.965
S(38)-C(37)-S(36)	117.8	H(57)-N(20)-C(18)	115.258	H(47)-C(6)-N(2)	108.919
C(37)-S(36)-C(23)	98.408	C(21)-N(20)-C(18)	124.5	H(46)-C(6)-N(2)	110.389
H(65)-N(35)-H(64)	108.377	C(18)-N(19)-C(15)	109.804	C(15)-C(5)-C(4)	125.06
H(65)-N(35)-S(32)	104.59	N(20)-C(18)-N(19)	119.492	C(15)-C(5)-C(1)	126.369
H(64)-N(35)-S(32)	105.694	N(20)-C(18)-S(17)	122.2	C(4)-C(5)-C(1)	108.536
N(35)-S(32)-O(34)	105.257	N(19)-C(18)-S(17)	118.278	O(14)-C(4)-C(5)	134.296
N(35)-S(32)-O(33)	108.495	C(18)-S(17)-C(16)	86.559	O(14)-C(4)-N(3)	122.576
N(35)-S(32)-C(29)	102.387	N(24)-C(16)-S(17)	124.586	C(5)-C(4)-N(3)	103.124
O(34)-S(32)-O(33)	122.946	N(24)-C(16)-C(15)	124.697	C(7)-N(3)-C(4)	126.424
O(34)-S(32)-C(29)	108.494	S(17)-C(16)-C(15)	110.584	C(7)-N(3)-N(2)	121.945
O(33)-S(32)-C(29)	107.403	N(19)-C(15)-C(16)	114.739	C(4)-N(3)-N(2)	111.001
H(63)-C(31)-C(30)	121.225	N(19)-C(15)-C(5)	121.404	C(6)-N(2)-N(3)	117.436
H(63)-C(31)-C(26)	118.417	C(16)-C(15)-C(5)	123.832	C(6)-N(2)-C(1)	127.072
C(30)-C(31)-C(26)	120.355	H(56)-C(13)-H(55)	107.427	N(3)-N(2)-C(1)	106.995
H(62)-C(30)-C(31)	120.952	H(56)-C(13)-H(54)	108.413	C(13)-C(1)-C(5)	128.431
H(62)-C(30)-C(29)	119.769	H(56)-C(13)-C(1)	109.853	C(13)-C(1)-N(2)	121.456
C(31)-C(30)-C(29)	119.276	H(55)-C(13)-H(54)	107.77	C(5)-C(1)-N(2)	110.109
S(32)-C(29)-C(30)	118.84	H(55)-C(13)-C(1)	110.635		
S(32)-C(29)-C(28)	120.158	H(54)-C(13)-C(1)	112.573		

Table S11. Bond lengths (Å) of compound **7b** using DFT-method from DMOL3 calculations

Bond	Length(Å)	Bond	Length(Å)	Bond	Length(Å)	Bond	Length(Å)
C(45)-H(69)	1.089	S(32)-O(33)	1.471	N(20)-H(57)	1.019	C(8)-H(49)	1.09
C(44)-H(68)	1.092	C(31)-H(63)	1.09	N(20)-C(21)	1.391	C(8)-C(9)	1.4
C(44)-C(45)	1.4	C(30)-H(62)	1.089	C(18)-N(20)	1.396	C(7)-C(12)	1.407
C(43)-H(67)	1.09	C(30)-C(31)	1.396	C(18)-N(19)	1.325	C(7)-C(8)	1.404
C(43)-C(44)	1.409	C(29)-S(32)	1.795	S(17)-C(18)	1.745	C(6)-H(48)	1.099
C(42)-H(66)	1.09	C(29)-C(30)	1.399	C(16)-N(24)	1.36	C(6)-H(47)	1.097
C(42)-C(43)	1.403	C(28)-H(61)	1.09	C(16)-S(17)	1.782	C(6)-H(46)	1.095
C(40)-C(45)	1.401	C(28)-C(29)	1.406	C(15)-N(19)	1.38	C(5)-C(15)	1.457
C(40)-N(41)	1.405	C(27)-H(60)	1.089	C(15)-C(16)	1.41	C(4)-O(14)	1.235
C(39)-C(42)	1.391	C(27)-C(28)	1.391	C(13)-H(56)	1.096	C(4)-C(5)	1.472
C(39)-C(40)	1.407	C(26)-C(31)	1.407	C(13)-H(55)	1.102	N(3)-C(7)	1.42
O(38)-C(39)	1.395	C(26)-C(27)	1.415	C(13)-H(54)	1.099	N(3)-C(4)	1.426
C(37)-N(41)	1.301	N(25)-C(26)	1.417	C(12)-H(53)	1.089	N(2)-C(6)	1.473
C(37)-O(38)	1.393	N(24)-N(25)	1.289	C(11)-H(52)	1.092	N(2)-N(3)	1.412
S(36)-C(37)	1.759	C(23)-H(59)	1.099	C(11)-C(12)	1.398	C(1)-C(13)	1.498
N(35)-H(65)	1.02	C(23)-H(58)	1.095	C(10)-H(51)	1.092	C(1)-C(5)	1.388
N(35)-H(64)	1.021	C(23)-S(36)	1.857	C(10)-C(11)	1.401	C(1)-N(2)	1.382
S(32)-N(35)	1.708	C(21)-C(23)	1.527	C(9)-H(50)	1.092		
S(32)-O(34)	1.47	C(21)-O(22)	1.232	C(9)-C(10)	1.401		

Table S12. Bond angles (°) of compound **7b** using DFT-method from DMOL3 calculations

Angle	Degree(°)	Angle	Degree(°)	Angle	Degree(°)
H(69)-C(45)-C(44)	122.272	C(30)-C(29)-C(28)	120.922	H(53)-C(12)-C(11)	121.178
H(69)-C(45)-C(40)	120.658	H(61)-C(28)-C(29)	120.074	H(53)-C(12)-C(7)	119.019
C(44)-C(45)-C(40)	117.069	H(61)-C(28)-C(27)	120.418	C(11)-C(12)-C(7)	119.801
H(68)-C(44)-C(45)	119.351	C(29)-C(28)-C(27)	119.481	H(52)-C(11)-C(12)	119.52
H(68)-C(44)-C(43)	118.789	H(60)-C(27)-C(28)	121.156	H(52)-C(11)-C(10)	120.156
C(45)-C(44)-C(43)	121.841	H(60)-C(27)-C(26)	118.543	C(12)-C(11)-C(10)	120.322
H(67)-C(43)-C(44)	118.953	C(28)-C(27)-C(26)	120.277	H(51)-C(10)-C(11)	119.786
H(67)-C(43)-C(42)	119.249	C(31)-C(26)-C(27)	119.438	H(51)-C(10)-C(9)	120.49
C(44)-C(43)-C(42)	121.794	C(31)-C(26)-N(25)	116.583	C(11)-C(10)-C(9)	119.716
H(66)-C(42)-C(43)	122.179	C(27)-C(26)-N(25)	123.878	H(50)-C(9)-C(10)	119.822
H(66)-C(42)-C(39)	122.55	C(26)-N(25)-N(24)	113.393	H(50)-C(9)-C(8)	119.728
C(43)-C(42)-C(39)	115.266	N(25)-N(24)-C(16)	116	C(10)-C(9)-C(8)	120.44
C(40)-N(41)-C(37)	103.705	H(59)-C(23)-H(58)	109.346	H(49)-C(8)-C(9)	120.831
C(45)-C(40)-N(41)	130.901	H(59)-C(23)-S(36)	108.639	H(49)-C(8)-C(7)	119.523
C(45)-C(40)-C(39)	119.854	H(59)-C(23)-C(21)	112.186	C(9)-C(8)-C(7)	119.646
N(41)-C(40)-C(39)	109.236	H(58)-C(23)-S(36)	108.6	C(12)-C(7)-C(8)	120.04
C(42)-C(39)-C(40)	124.122	H(58)-C(23)-C(21)	107.365	C(12)-C(7)-N(3)	118.493
C(42)-C(39)-O(38)	128.218	S(36)-C(23)-C(21)	110.635	C(8)-C(7)-N(3)	121.466
C(40)-C(39)-O(38)	107.649	C(23)-C(21)-O(22)	122.104	H(48)-C(6)-H(47)	108.458
C(39)-O(38)-C(37)	102.744	C(23)-C(21)-N(20)	115.61	H(48)-C(6)-H(46)	109.219
N(41)-C(37)-O(38)	116.66	O(22)-C(21)-N(20)	122.146	H(48)-C(6)-N(2)	111.608
N(41)-C(37)-S(36)	128.68	H(57)-N(20)-C(21)	119.765	H(47)-C(6)-H(46)	108.544
O(38)-C(37)-S(36)	114.657	H(57)-N(20)-C(18)	115.392	H(47)-C(6)-N(2)	109.246
C(37)-S(36)-C(23)	96.665	C(21)-N(20)-C(18)	124.757	H(46)-C(6)-N(2)	109.705
H(65)-N(35)-H(64)	110.7	C(18)-N(19)-C(15)	110.032	C(15)-C(5)-C(4)	124.599
H(65)-N(35)-S(32)	109.187	N(20)-C(18)-N(19)	119.63	C(15)-C(5)-C(1)	127.473
H(64)-N(35)-S(32)	108.057	N(20)-C(18)-S(17)	122.163	C(4)-C(5)-C(1)	107.921
N(35)-S(32)-O(34)	105.681	N(19)-C(18)-S(17)	118.207	O(14)-C(4)-C(5)	133.055
N(35)-S(32)-O(33)	108.91	C(18)-S(17)-C(16)	86.596	O(14)-C(4)-N(3)	122.939
N(35)-S(32)-C(29)	101.91	N(24)-C(16)-S(17)	124.329	C(5)-C(4)-N(3)	104.002
O(34)-S(32)-O(33)	123.087	N(24)-C(16)-C(15)	124.958	C(7)-N(3)-C(4)	126.494
O(34)-S(32)-C(29)	108.777	S(17)-C(16)-C(15)	110.663	C(7)-N(3)-N(2)	122.101
O(33)-S(32)-C(29)	106.518	N(19)-C(15)-C(16)	114.476	C(4)-N(3)-N(2)	109.983
H(63)-C(31)-C(30)	121.135	N(19)-C(15)-C(5)	121.67	C(6)-N(2)-N(3)	117.233
H(63)-C(31)-C(26)	118.475	C(16)-C(15)-C(5)	123.839	C(6)-N(2)-C(1)	124.175
C(30)-C(31)-C(26)	120.389	H(56)-C(13)-H(55)	107.288	N(3)-N(2)-C(1)	107.216
H(62)-C(30)-C(31)	120.923	H(56)-C(13)-H(54)	108.736	C(13)-C(1)-C(5)	128.691
H(62)-C(30)-C(29)	119.579	H(56)-C(13)-C(1)	109.821	C(13)-C(1)-N(2)	120.958
C(31)-C(30)-C(29)	119.483	H(55)-C(13)-H(54)	107.923	C(5)-C(1)-N(2)	110.335
S(32)-C(29)-C(30)	118.728	H(55)-C(13)-C(1)	110.265		
S(32)-C(29)-C(28)	120.287	H(54)-C(13)-C(1)	112.641		

Table S13. Bond lengths (Å) of compound **9** using DFT-method from DMOL3 calculations

Bond	Length(Å)	Bond	Length(Å)	Bond	Length(Å)	Bond	Length(Å)
N(25)-H(41)	1.017	C(18)-N(19)	1.319	C(11)-C(12)	1.399	C(6)-H(27)	1.099
C(24)-O(26)	1.226	S(17)-C(18)	1.794	C(10)-H(32)	1.093	C(5)-C(13)	1.501
C(24)-N(25)	1.386	C(16)-H(38)	1.084	C(10)-C(11)	1.401	C(4)-C(15)	1.465
C(23)-H(40)	1.099	C(16)-S(17)	1.724	C(9)-H(31)	1.092	C(4)-C(5)	1.387
C(23)-H(39)	1.099	C(15)-N(19)	1.381	C(9)-C(10)	1.401	C(3)-O(14)	1.238
C(23)-C(24)	1.533	C(15)-C(16)	1.39	C(8)-H(30)	1.091	C(3)-C(4)	1.467
S(22)-C(23)	1.842	C(13)-H(37)	1.104	C(8)-C(9)	1.4	N(2)-C(7)	1.426
C(21)-N(25)	1.397	C(13)-H(36)	1.102	C(7)-C(12)	1.408	N(2)-C(3)	1.428
C(21)-S(22)	1.791	C(13)-H(35)	1.095	C(7)-C(8)	1.406	N(1)-C(6)	1.479
N(20)-C(21)	1.287	C(12)-H(34)	1.089	C(6)-H(29)	1.093	N(1)-C(5)	1.397
C(18)-N(20)	1.375	C(11)-H(33)	1.094	C(6)-H(28)	1.1	N(1)-N(2)	1.414

Table S14. Bond angles (°) of compound **9** using DFT-method from DMOL3 calculations

Angle	Degree(°)	Angle	Degree(°)	Angle	Degree(°)
H(41)-N(25)-C(24)	120.928	N(19)-C(15)-C(16)	114.936	C(12)-C(7)-N(2)	118.601
H(41)-N(25)-C(21)	119.116	N(19)-C(15)-C(4)	120.916	C(8)-C(7)-N(2)	121.617
C(24)-N(25)-C(21)	119.955	C(16)-C(15)-C(4)	124.148	H(29)-C(6)-H(28)	109.163
O(26)-C(24)-N(25)	125.268	H(37)-C(13)-H(36)	107.879	H(29)-C(6)-H(27)	108.899
O(26)-C(24)-C(23)	124.906	H(37)-C(13)-H(35)	107.989	H(29)-C(6)-N(1)	109.272
N(25)-C(24)-C(23)	109.825	H(37)-C(13)-C(5)	111.985	H(28)-C(6)-H(27)	108.867
H(40)-C(23)-H(39)	108.972	H(36)-C(13)-H(35)	109.395	H(28)-C(6)-N(1)	109.973
H(40)-C(23)-C(24)	109.634	H(36)-C(13)-C(5)	110.893	H(27)-C(6)-N(1)	110.64
H(40)-C(23)-S(22)	110.33	H(35)-C(13)-C(5)	108.634	C(13)-C(5)-C(4)	129.858
H(39)-C(23)-C(24)	109.264	H(34)-C(12)-C(11)	120.962	C(13)-C(5)-N(1)	119.951
H(39)-C(23)-S(22)	110.355	H(34)-C(12)-C(7)	119.135	C(4)-C(5)-N(1)	110.184
C(24)-C(23)-S(22)	108.269	C(11)-C(12)-C(7)	119.885	C(15)-C(4)-C(5)	129.693
C(23)-S(22)-C(21)	92.01	H(33)-C(11)-C(12)	119.243	C(15)-C(4)-C(3)	122.247
N(25)-C(21)-S(22)	109.861	H(33)-C(11)-C(10)	120.266	C(5)-C(4)-C(3)	108.048
N(25)-C(21)-N(20)	119.614	C(12)-C(11)-C(10)	120.487	O(14)-C(3)-C(4)	131.503
S(22)-C(21)-N(20)	130.526	H(32)-C(10)-C(11)	120.318	O(14)-C(3)-N(2)	123.847
C(21)-N(20)-C(18)	125.184	H(32)-C(10)-C(9)	120.203	C(4)-C(3)-N(2)	104.633
C(18)-N(19)-C(15)	112.207	C(11)-C(10)-C(9)	119.465	C(7)-N(2)-C(3)	125.331
N(20)-C(18)-N(19)	120.99	H(31)-C(9)-C(10)	119.868	C(7)-N(2)-N(1)	120.156
N(20)-C(18)-S(17)	125.969	H(31)-C(9)-C(8)	119.509	C(3)-N(2)-N(1)	109.876
N(19)-C(18)-S(17)	113.033	C(10)-C(9)-C(8)	120.617	C(6)-N(1)-C(5)	122.641
C(18)-S(17)-C(16)	88.991	H(30)-C(8)-C(9)	120.532	C(6)-N(1)-N(2)	115.089
H(38)-C(16)-S(17)	121.695	H(30)-C(8)-C(7)	119.626	C(5)-N(1)-N(2)	106.856
H(38)-C(16)-C(15)	127.533	C(9)-C(8)-C(7)	119.748		

Table S15. Bond lengths (Å) of compound **10a** using DFT-method from DMOL3 calculations

Bond	Length(Å)	Bond	Length(Å)	Bond	Length(Å)	Bond	Length(Å)
C(35)-H(56)	1.104	C(27)-H(49)	1.095	C(16)-S(17)	1.729	C(7)-C(12)	1.41
C(35)-H(55)	1.102	C(27)-C(28)	1.454	C(15)-N(19)	1.389	C(7)-C(8)	1.409
C(35)-H(54)	1.096	N(25)-H(48)	1.017	C(15)-C(16)	1.385	C(6)-H(38)	1.098
O(34)-C(35)	1.44	C(24)-O(26)	1.231	C(13)-H(46)	1.095	C(6)-H(37)	1.098
C(33)-H(53)	1.092	C(24)-N(25)	1.407	C(13)-H(45)	1.1	C(6)-H(36)	1.093
C(32)-H(52)	1.091	C(23)-C(27)	1.365	C(13)-H(44)	1.102	C(5)-C(13)	1.5
C(32)-C(33)	1.389	C(23)-C(24)	1.49	C(12)-H(43)	1.087	C(4)-C(15)	1.463
C(31)-O(34)	1.376	S(22)-C(23)	1.778	C(11)-H(42)	1.094	C(4)-C(5)	1.38
C(31)-C(32)	1.413	C(21)-N(25)	1.382	C(11)-C(12)	1.4	C(3)-O(14)	1.24
C(30)-H(51)	1.09	C(21)-S(22)	1.794	C(10)-H(41)	1.093	C(3)-C(4)	1.464
C(30)-C(31)	1.407	N(20)-C(21)	1.298	C(10)-C(11)	1.401	N(2)-C(7)	1.429
C(29)-H(50)	1.09	C(18)-N(20)	1.388	C(9)-H(40)	1.091	N(2)-C(3)	1.428
C(29)-C(30)	1.396	C(18)-N(19)	1.322	C(9)-C(10)	1.403	N(1)-C(6)	1.477
C(28)-C(33)	1.422	S(17)-C(18)	1.767	C(8)-H(39)	1.091	N(1)-C(5)	1.401
C(28)-C(29)	1.416	C(16)-H(47)	1.086	C(8)-C(9)	1.399	N(1)-N(2)	1.417

Table S16. Bond angles (°) of compound **10a** using DFT-method from DMOL3 calculations

Angle	Degree(°)	Angle	Degree(°)	Angle	Degree(°)
H(56)-C(35)-H(55)	110.195	N(25)-C(24)-C(23)	108.521	H(41)-C(10)-C(9)	120.077
H(56)-C(35)-H(54)	109.532	C(27)-C(23)-C(24)	121.434	C(11)-C(10)-C(9)	119.415
H(56)-C(35)-O(34)	110.657	C(27)-C(23)-S(22)	127.367	H(40)-C(9)-C(10)	119.786
H(55)-C(35)-H(54)	109.164	C(24)-C(23)-S(22)	111.191	H(40)-C(9)-C(8)	119.244
H(55)-C(35)-O(34)	111.576	C(23)-S(22)-C(21)	91.391	C(10)-C(9)-C(8)	120.933
H(54)-C(35)-O(34)	105.596	N(25)-C(21)-S(22)	109.548	H(39)-C(8)-C(9)	120.131
C(35)-O(34)-C(31)	117.53	N(25)-C(21)-N(20)	122.695	H(39)-C(8)-C(7)	120.371
H(53)-C(33)-C(32)	119.566	S(22)-C(21)-N(20)	127.557	C(9)-C(8)-C(7)	119.476
H(53)-C(33)-C(28)	119.158	C(21)-N(20)-C(18)	118.016	C(12)-C(7)-C(8)	119.722
C(32)-C(33)-C(28)	121.258	C(18)-N(19)-C(15)	110.742	C(12)-C(7)-N(2)	119.454
H(52)-C(32)-C(33)	121.302	N(20)-C(18)-N(19)	126.524	C(8)-C(7)-N(2)	120.823
H(52)-C(32)-C(31)	118.783	N(20)-C(18)-S(17)	118.642	H(38)-C(6)-H(37)	109.192
C(33)-C(32)-C(31)	119.897	N(19)-C(18)-S(17)	114.8	H(38)-C(6)-H(36)	109.082
O(34)-C(31)-C(32)	116.383	C(18)-S(17)-C(16)	88.58	H(38)-C(6)-N(1)	109.796
O(34)-C(31)-C(30)	123.571	H(47)-C(16)-S(17)	121.587	H(37)-C(6)-H(36)	108.893
C(32)-C(31)-C(30)	120.044	H(47)-C(16)-C(15)	127.396	H(37)-C(6)-N(1)	110.658
H(51)-C(30)-C(31)	121.154	S(17)-C(16)-C(15)	110.95	H(36)-C(6)-N(1)	109.192
H(51)-C(30)-C(29)	119.438	N(19)-C(15)-C(16)	114.925	C(13)-C(5)-C(4)	128.032
C(31)-C(30)-C(29)	119.401	N(19)-C(15)-C(4)	121.195	C(13)-C(5)-N(1)	122.278
H(50)-C(29)-C(30)	118.036	C(16)-C(15)-C(4)	123.854	C(4)-C(5)-N(1)	109.659
H(50)-C(29)-C(28)	120.141	H(46)-C(13)-H(45)	108.28	C(15)-C(4)-C(5)	129.74
C(30)-C(29)-C(28)	121.716	H(46)-C(13)-H(44)	108.648	C(15)-C(4)-C(3)	122.072
C(33)-C(28)-C(29)	117.644	H(46)-C(13)-C(5)	109.375	C(5)-C(4)-C(3)	108.106
C(33)-C(28)-C(27)	118.789	H(45)-C(13)-H(44)	107.44	O(14)-C(3)-C(4)	129.858
C(29)-C(28)-C(27)	123.464	H(45)-C(13)-C(5)	112.67	O(14)-C(3)-N(2)	124.693
H(49)-C(27)-C(28)	116.056	H(44)-C(13)-C(5)	110.323	C(4)-C(3)-N(2)	105.449
H(49)-C(27)-C(23)	113.427	H(43)-C(12)-C(11)	120.594	C(7)-N(2)-C(3)	125.18
C(28)-C(27)-C(23)	130.498	H(43)-C(12)-C(7)	119.316	C(7)-N(2)-N(1)	120.384
H(48)-N(25)-C(24)	120.605	C(11)-C(12)-C(7)	120.086	C(3)-N(2)-N(1)	108.461
H(48)-N(25)-C(21)	120.414	H(42)-C(11)-C(12)	119.133	C(6)-N(1)-C(5)	122.989
C(24)-N(25)-C(21)	118.853	H(42)-C(11)-C(10)	120.527	C(6)-N(1)-N(2)	114.52
O(26)-C(24)-N(25)	123.219	C(12)-C(11)-C(10)	120.32	C(5)-N(1)-N(2)	107.72
O(26)-C(24)-C(23)	128.013	H(41)-C(10)-C(11)	120.506		

Table S17. Bond lengths (Å) of compound **10b** using DFT-method from DMOL3 calculations

Bond	Length(Å)	Bond	Length(Å)	Bond	Length(Å)	Bond	Length(Å)
N(34)-O(36)	1.244	N(25)-H(49)	1.017	C(15)-C(16)	1.391	C(6)-H(39)	1.103
N(34)-O(35)	1.243	C(24)-O(26)	1.229	C(13)-H(47)	1.103	C(6)-H(38)	1.095
C(33)-H(54)	1.091	C(24)-N(25)	1.398	C(13)-H(46)	1.1	C(6)-H(37)	1.095
C(32)-H(53)	1.088	C(23)-C(27)	1.363	C(13)-H(45)	1.095	C(5)-C(13)	1.5
C(32)-C(33)	1.39	C(23)-C(24)	1.498	C(12)-H(44)	1.09	C(4)-C(15)	1.462
C(31)-N(34)	1.482	S(22)-C(23)	1.772	C(11)-H(43)	1.091	C(4)-C(5)	1.384
C(31)-C(32)	1.403	C(21)-N(25)	1.382	C(11)-C(12)	1.397	C(3)-O(14)	1.236
C(30)-H(52)	1.088	C(21)-S(22)	1.797	C(10)-H(42)	1.091	C(3)-C(4)	1.47
C(30)-C(31)	1.404	N(20)-C(21)	1.293	C(10)-C(11)	1.403	N(2)-C(7)	1.427
C(29)-H(51)	1.091	C(18)-N(20)	1.376	C(9)-H(41)	1.093	N(2)-C(3)	1.429
C(29)-C(30)	1.393	C(18)-N(19)	1.322	C(9)-C(10)	1.402	N(1)-C(6)	1.475
C(28)-C(33)	1.42	S(17)-C(18)	1.763	C(8)-H(40)	1.091	N(1)-C(5)	1.396
C(28)-C(29)	1.418	C(16)-H(48)	1.085	C(8)-C(9)	1.399	N(1)-N(2)	1.416
C(27)-H(50)	1.094	C(16)-S(17)	1.725	C(7)-C(12)	1.407		
C(27)-C(28)	1.455	C(15)-N(19)	1.387	C(7)-C(8)	1.409		

Table S18. Bond angles (°) of compound **10b** using DFT-method from DMOL3 calculations

Angle	Degree(°)	Angle	Degree(°)	Angle	Degree(°)
O(36)-N(34)-O(35)	124.531	C(24)-C(23)-S(22)	111.441	H(41)-C(9)-C(10)	120.083
O(36)-N(34)-C(31)	117.915	C(23)-S(22)-C(21)	91.227	H(41)-C(9)-C(8)	119.561
O(35)-N(34)-C(31)	117.553	N(25)-C(21)-S(22)	109.753	C(10)-C(9)-C(8)	120.348
H(54)-C(33)-C(32)	119.574	N(25)-C(21)-N(20)	121.083	H(40)-C(8)-C(9)	120.394
H(54)-C(33)-C(28)	119.097	S(22)-C(21)-N(20)	129.127	H(40)-C(8)-C(7)	119.906
C(32)-C(33)-C(28)	121.323	C(21)-N(20)-C(18)	121.426	C(9)-C(8)-C(7)	119.677
H(53)-C(32)-C(33)	121.429	C(18)-N(19)-C(15)	111.17	C(12)-C(7)-C(8)	120.188
H(53)-C(32)-C(31)	119.512	N(20)-C(18)-N(19)	127.445	C(12)-C(7)-N(2)	118.25
C(33)-C(32)-C(31)	119.053	N(20)-C(18)-S(17)	118.038	C(8)-C(7)-N(2)	121.558
N(34)-C(31)-C(32)	119.232	N(19)-C(18)-S(17)	114.437	H(39)-C(6)-H(38)	109.451
N(34)-C(31)-C(30)	119.584	C(18)-S(17)-C(16)	88.988	H(39)-C(6)-H(37)	110.118
C(32)-C(31)-C(30)	121.184	H(48)-C(16)-S(17)	122.586	H(39)-C(6)-N(1)	111.645
H(52)-C(30)-C(31)	119.376	H(48)-C(16)-C(15)	126.693	H(38)-C(6)-H(37)	108.559
H(52)-C(30)-C(29)	121.265	S(17)-C(16)-C(15)	110.72	H(38)-C(6)-N(1)	108.576
C(31)-C(30)-C(29)	119.347	N(19)-C(15)-C(16)	114.662	H(37)-C(6)-N(1)	108.424
H(51)-C(29)-C(30)	118.716	N(19)-C(15)-C(4)	121.575	C(13)-C(5)-C(4)	130.497
H(51)-C(29)-C(28)	120.328	C(16)-C(15)-C(4)	123.737	C(13)-C(5)-N(1)	119.147
C(30)-C(29)-C(28)	120.909	H(47)-C(13)-H(46)	108.086	C(4)-C(5)-N(1)	110.347
C(33)-C(28)-C(29)	118.179	H(47)-C(13)-H(45)	107.438	C(15)-C(4)-C(5)	129.824
C(33)-C(28)-C(27)	117.166	H(47)-C(13)-C(5)	111.501	C(15)-C(4)-C(3)	122.03
C(29)-C(28)-C(27)	124.645	H(46)-C(13)-H(45)	109.278	C(5)-C(4)-C(3)	107.857
H(50)-C(27)-C(28)	115.39	H(46)-C(13)-C(5)	110.901	O(14)-C(3)-C(4)	131.207
H(50)-C(27)-C(23)	113.243	H(45)-C(13)-C(5)	109.547	O(14)-C(3)-N(2)	124.016
C(28)-C(27)-C(23)	131.361	H(44)-C(12)-C(11)	121.101	C(4)-C(3)-N(2)	104.763
H(49)-N(25)-C(24)	121.18	H(44)-C(12)-C(7)	119.432	C(7)-N(2)-C(3)	124.152
H(49)-N(25)-C(21)	119.929	C(11)-C(12)-C(7)	119.46	C(7)-N(2)-N(1)	119.632
C(24)-N(25)-C(21)	118.885	H(43)-C(11)-C(12)	119.022	C(3)-N(2)-N(1)	109.437
O(26)-C(24)-N(25)	124.369	H(43)-C(11)-C(10)	120.262	C(6)-N(1)-C(5)	120.507
O(26)-C(24)-C(23)	127.137	C(12)-C(11)-C(10)	120.713	C(6)-N(1)-N(2)	114.328
N(25)-C(24)-C(23)	108.493	H(42)-C(10)-C(11)	120.111	C(5)-N(1)-N(2)	106.965
C(27)-C(23)-C(24)	119.283	H(42)-C(10)-C(9)	120.3		
C(27)-C(23)-S(22)	129.178	C(11)-C(10)-C(9)	119.587		

Table S19. Bond lengths (Å) of compound **10c** using DFT-method from DMOL3 calculations

Bond	Length(Å)	Bond	Length(Å)	Bond	Length(Å)	Bond	Length(Å)
C(33)-H(52)	1.092	C(24)-O(26)	1.227	C(15)-C(16)	1.385	C(7)-C(8)	1.405
C(32)-H(51)	1.09	C(24)-N(25)	1.403	C(13)-H(45)	1.094	C(6)-H(37)	1.103
C(32)-C(33)	1.394	C(23)-C(27)	1.363	C(13)-H(44)	1.106	C(6)-H(36)	1.098
C(31)-Br(34)	1.919	C(23)-C(24)	1.499	C(13)-H(43)	1.101	C(6)-H(35)	1.095
C(31)-C(32)	1.404	S(22)-C(23)	1.775	C(12)-H(42)	1.089	C(5)-C(13)	1.496
C(30)-H(50)	1.09	C(21)-N(25)	1.38	C(11)-H(41)	1.092	C(4)-C(15)	1.462
C(30)-C(31)	1.403	C(21)-S(22)	1.793	C(11)-C(12)	1.398	C(4)-C(5)	1.385
C(29)-H(49)	1.09	N(20)-C(21)	1.289	C(10)-H(40)	1.092	C(3)-O(14)	1.237
C(29)-C(30)	1.396	C(18)-N(20)	1.4	C(10)-C(11)	1.401	C(3)-C(4)	1.467
C(28)-C(33)	1.417	C(18)-N(19)	1.311	C(9)-H(39)	1.092	N(2)-C(7)	1.429
C(28)-C(29)	1.416	S(17)-C(18)	1.778	C(9)-C(10)	1.403	N(2)-C(3)	1.426
C(27)-H(48)	1.094	C(16)-H(46)	1.087	C(8)-H(38)	1.091	N(1)-C(6)	1.472
C(27)-C(28)	1.455	C(16)-S(17)	1.728	C(8)-C(9)	1.4	N(1)-C(5)	1.396
N(25)-H(47)	1.015	C(15)-N(19)	1.394	C(7)-C(12)	1.405	N(1)-N(2)	1.418

Table S20. Bond angles (°) of compound **10c** using DFT-method from DMOL3 calculations

Angle	Degree(°)	Angle	Degree(°)	Angle	Degree(°)
H(52)-C(33)-C(32)	119.317	N(25)-C(21)-S(22)	110.058	H(39)-C(9)-C(8)	119.468
H(52)-C(33)-C(28)	119.183	N(25)-C(21)-N(20)	123.421	C(10)-C(9)-C(8)	120.131
C(32)-C(33)-C(28)	121.496	S(22)-C(21)-N(20)	126.517	H(38)-C(8)-C(9)	120.666
H(51)-C(32)-C(33)	120.531	C(21)-N(20)-C(18)	117.398	H(38)-C(8)-C(7)	119.368
H(51)-C(32)-C(31)	120.375	C(18)-N(19)-C(15)	111.05	C(9)-C(8)-C(7)	119.963
C(33)-C(32)-C(31)	119.092	N(20)-C(18)-N(19)	124.635	C(12)-C(7)-C(8)	120.07
Br(34)-C(31)-C(32)	118.764	N(20)-C(18)-S(17)	120.905	C(12)-C(7)-N(2)	118.62
Br(34)-C(31)-C(30)	120.232	N(19)-C(18)-S(17)	114.456	C(8)-C(7)-N(2)	121.301
C(32)-C(31)-C(30)	120.942	C(18)-S(17)-C(16)	88.703	H(37)-C(6)-H(36)	109.675
H(50)-C(30)-C(31)	120.209	H(46)-C(16)-S(17)	121.927	H(37)-C(6)-H(35)	109.818
H(50)-C(30)-C(29)	120.416	H(46)-C(16)-C(15)	127.345	H(37)-C(6)-N(1)	111.674
C(31)-C(30)-C(29)	119.364	S(17)-C(16)-C(15)	110.719	H(36)-C(6)-H(35)	108.635
H(49)-C(29)-C(30)	118.492	N(19)-C(15)-C(16)	115.038	H(36)-C(6)-N(1)	108.576
H(49)-C(29)-C(28)	120.316	N(19)-C(15)-C(4)	120.561	H(35)-C(6)-N(1)	108.398
C(30)-C(29)-C(28)	121.162	C(16)-C(15)-C(4)	124.346	C(13)-C(5)-C(4)	130.482
C(33)-C(28)-C(29)	117.94	H(45)-C(13)-H(44)	107.122	C(13)-C(5)-N(1)	119.44
C(33)-C(28)-C(27)	117.806	H(45)-C(13)-H(43)	109.898	C(4)-C(5)-N(1)	110.077
C(29)-C(28)-C(27)	124.253	H(45)-C(13)-C(5)	109.596	C(15)-C(4)-C(5)	128.956
H(48)-C(27)-C(28)	115.84	H(44)-C(13)-H(43)	107.602	C(15)-C(4)-C(3)	122.884
H(48)-C(27)-C(23)	113.336	H(44)-C(13)-C(5)	111.381	C(5)-C(4)-C(3)	108.159
C(28)-C(27)-C(23)	130.781	H(43)-C(13)-C(5)	111.142	O(14)-C(3)-C(4)	131.61
H(47)-N(25)-C(24)	121.05	H(42)-C(12)-C(11)	121.121	O(14)-C(3)-N(2)	123.862
H(47)-N(25)-C(21)	120.359	H(42)-C(12)-C(7)	119.404	C(4)-C(3)-N(2)	104.512
C(24)-N(25)-C(21)	118.538	C(11)-C(12)-C(7)	119.472	C(7)-N(2)-C(3)	124.943
O(26)-C(24)-N(25)	123.803	H(41)-C(11)-C(12)	119.295	C(7)-N(2)-N(1)	119.176
O(26)-C(24)-C(23)	127.406	H(41)-C(11)-C(10)	119.948	C(3)-N(2)-N(1)	109.571
N(25)-C(24)-C(23)	108.791	C(12)-C(11)-C(10)	120.748	C(6)-N(1)-C(5)	121.423
C(27)-C(23)-C(24)	120.854	H(40)-C(10)-C(11)	119.99	C(6)-N(1)-N(2)	114.491
C(27)-C(23)-S(22)	127.981	H(40)-C(10)-C(9)	120.411	C(5)-N(1)-N(2)	106.732
C(24)-C(23)-S(22)	111.131	C(11)-C(10)-C(9)	119.599		
C(23)-S(22)-C(21)	91.422	H(39)-C(9)-C(10)	120.394		

Table S21. Bond lengths (Å) of compound **12** using DFT-method from DMOL3 calculations

Bond	Length	Bond	Length	Bond	Length	Bond	Length
C(27)-N(28)	1.171	C(19)-N(20)	1.337	C(14)-H(31)	1.101	N(7)-N(8)	1.381
C(26)-H(44)	1.09	C(18)-C(27)	1.388	C(14)-H(30)	1.103	C(6)-H(29)	1.092
C(25)-H(43)	1.093	C(18)-C(19)	1.366	C(26)-C(12)	1.391	C(5)-C(10)	1.429
C(25)-C(26)	1.384	C(17)-H(37)	1.104	C(12)-C(22)	1.391	C(5)-C(6)	1.375
C(24)-H(42)	1.093	C(17)-H(36)	1.104	C(11)-C(14)	1.467	N(4)-C(5)	1.363
C(24)-C(25)	1.387	C(17)-C(18)	1.487	C(10)-C(11)	1.373	C(3)-N(4)	1.292
C(23)-H(41)	1.092	C(16)-O(21)	1.208	C(9)-O(13)	1.231	S(2)-C(6)	1.697
C(23)-C(24)	1.386	C(16)-C(17)	1.503	C(9)-C(10)	1.435	S(2)-C(3)	1.743
C(22)-H(40)	1.093	C(15)-H(35)	1.102	N(8)-C(12)	1.396	C(19)-N(1)	1.389
C(22)-C(23)	1.384	C(15)-H(34)	1.1	N(8)-C(9)	1.411	N(1)-C(16)	1.418
N(20)-H(39)	1.018	C(15)-H(33)	1.099	N(7)-C(15)	1.443	N(1)-C(3)	1.38
N(20)-H(38)	1.021	C(14)-H(32)	1.107	N(7)-C(11)	1.362	N(7)-N(8)	1.381

Table S22. Bond angles (°) of compound **12** using DFT-method from DMOL3 calculations

Angle	Degree	Angle	Degree	Angle	Degree
N(28)-C(27)-C(18)	176.406	H(37)-C(17)-C(18)	114.053	C(11)-C(10)-C(9)	108.217
H(44)-C(26)-C(25)	121.788	H(37)-C(17)-C(16)	108.917	C(11)-C(10)-C(5)	128.687
H(44)-C(26)-C(12)	119.087	H(36)-C(17)-C(18)	114.564	C(9)-C(10)-C(5)	122.926
C(25)-C(26)-C(12)	119.109	H(36)-C(17)-C(16)	108.519	O(13)-C(9)-C(10)	130.964
H(43)-C(25)-C(26)	119.135	C(18)-C(17)-C(16)	104.071	O(13)-C(9)-N(8)	124.216
H(43)-C(25)-C(24)	120.068	O(21)-C(16)-C(17)	128.752	C(10)-C(9)-N(8)	104.741
C(26)-C(25)-C(24)	120.786	O(21)-C(16)-N(1)	124.893	C(12)-N(8)-C(9)	123.744
H(42)-C(24)-C(25)	120.256	C(17)-C(16)-N(1)	106.346	C(12)-N(8)-N(7)	119.494
H(42)-C(24)-C(23)	120.115	H(35)-C(15)-H(34)	108.868	C(9)-N(8)-N(7)	109.158
C(25)-C(24)-C(23)	119.629	H(35)-C(15)-H(33)	108.347	C(15)-N(7)-C(11)	123.349
H(41)-C(23)-C(24)	120.395	H(35)-C(15)-N(7)	112.455	C(15)-N(7)-N(8)	118.623
H(41)-C(23)-C(22)	119.263	H(34)-C(15)-H(33)	108.739	C(11)-N(7)-N(8)	108.323
C(24)-C(23)-C(22)	120.331	H(34)-C(15)-N(7)	109.211	H(29)-C(6)-C(5)	125.321
H(40)-C(22)-C(23)	120.757	H(33)-C(15)-N(7)	109.151	H(29)-C(6)-S(2)	124.604
H(40)-C(22)-C(12)	119.592	H(32)-C(14)-H(31)	107.292	C(5)-C(6)-S(2)	110.046
C(23)-C(22)-C(12)	119.6	H(32)-C(14)-H(30)	107.765	C(10)-C(5)-C(6)	123.994
H(39)-N(20)-H(38)	120.659	H(32)-C(14)-C(11)	111.226	C(10)-C(5)-N(4)	120.839
H(39)-N(20)-C(19)	117.919	H(31)-C(14)-H(30)	110.268	C(6)-C(5)-N(4)	115.149
H(38)-N(20)-C(19)	121.171	H(31)-C(14)-C(11)	110.842	C(5)-N(4)-C(3)	111.191
N(20)-C(19)-C(18)	128.343	H(30)-C(14)-C(11)	109.386	N(4)-C(3)-S(2)	114.364
N(20)-C(19)-N(1)	121.104	C(26)-C(12)-C(22)	120.534	N(4)-C(3)-N(1)	122.979
C(18)-C(19)-N(1)	110.553	C(26)-C(12)-N(8)	119.022	S(2)-C(3)-N(1)	122.597
C(27)-C(18)-C(19)	121.765	C(22)-C(12)-N(8)	120.425	C(6)-S(2)-C(3)	89.143
C(27)-C(18)-C(17)	129.273	C(14)-C(11)-C(10)	130.145	C(19)-N(1)-C(16)	110.09
C(19)-C(18)-C(17)	108.93	C(14)-C(11)-N(7)	120.454	C(19)-N(1)-C(3)	126.359
H(37)-C(17)-H(36)	106.52	C(10)-C(11)-N(7)	109.391	C(16)-N(1)-C(3)	123.507

Table S23. Bond lengths (Å) of compound **14** using DFT-method from DMOL3 calculations

Bond	Length(Å)	Bond	Length(Å)	Bond	Length(Å)	Bond	Length(Å)
C(31)-H(49)	1.09	C(23)-O(24)	1.387	C(14)-H(40)	1.095	C(7)-C(8)	1.408
C(30)-H(48)	1.091	C(21)-C(23)	1.48	C(13)-H(39)	1.103	N(5)-C(7)	1.424
C(30)-C(31)	1.394	C(21)-O(22)	1.237	C(13)-H(38)	1.097	N(4)-C(13)	1.478
C(29)-H(47)	1.089	N(20)-H(44)	1.015	C(13)-H(37)	1.096	N(4)-N(5)	1.418
C(29)-C(30)	1.414	N(20)-C(21)	1.391	C(12)-H(36)	1.087	C(3)-C(14)	1.497
C(28)-H(46)	1.089	C(18)-N(20)	1.396	C(11)-H(35)	1.091	C(3)-N(4)	1.402
C(28)-C(29)	1.401	C(18)-N(19)	1.317	C(11)-C(12)	1.397	C(2)-C(15)	1.463
C(27)-H(45)	1.087	S(17)-C(18)	1.747	C(10)-H(34)	1.09	C(2)-C(3)	1.38
C(26)-C(31)	1.412	C(16)-H(43)	1.084	C(10)-C(11)	1.402	C(1)-O(6)	1.239
C(26)-C(27)	1.436	C(16)-S(17)	1.732	C(9)-H(33)	1.092	C(1)-N(5)	1.425
C(25)-C(28)	1.394	C(15)-N(19)	1.393	C(9)-C(10)	1.399	C(1)-C(2)	1.47
C(25)-C(26)	1.415	C(15)-C(16)	1.385	C(8)-H(32)	1.091		
O(24)-C(25)	1.379	C(14)-H(42)	1.106	C(8)-C(9)	1.399		
C(23)-C(27)	1.38	C(14)-H(41)	1.103	C(7)-C(12)	1.406		

Table S24. Bond angles (°) of compound **14** using DFT-method from DMOL3 calculations

Angle	Degree(°)	Angle	Degree(°)	Angle	Degree(°)
H(49)-C(31)-C(30)	120.732	H(44)-N(20)-C(18)	114.578	H(35)-C(11)-C(10)	119.809
H(49)-C(31)-C(26)	120.992	C(21)-N(20)-C(18)	124.341	C(12)-C(11)-C(10)	120.669
C(30)-C(31)-C(26)	118.276	C(18)-N(19)-C(15)	109.86	H(34)-C(10)-C(11)	120.244
H(48)-C(30)-C(31)	119.408	N(20)-C(18)-N(19)	120.574	H(34)-C(10)-C(9)	120.159
H(48)-C(30)-C(29)	119.081	N(20)-C(18)-S(17)	123.041	C(11)-C(10)-C(9)	119.597
C(31)-C(30)-C(29)	121.511	N(19)-C(18)-S(17)	116.371	H(33)-C(9)-C(10)	120.317
H(47)-C(29)-C(30)	119.476	C(18)-S(17)-C(16)	88.016	H(33)-C(9)-C(8)	119.241
H(47)-C(29)-C(28)	119.233	H(43)-C(16)-S(17)	121.767	C(10)-C(9)-C(8)	120.432
C(30)-C(29)-C(28)	121.292	H(43)-C(16)-C(15)	127.056	H(32)-C(8)-C(9)	120.911
H(46)-C(28)-C(29)	122.444	S(17)-C(16)-C(15)	111.157	H(32)-C(8)-C(7)	119.405
H(46)-C(28)-C(25)	121.147	N(19)-C(15)-C(16)	114.589	C(9)-C(8)-C(7)	119.672
C(29)-C(28)-C(25)	116.408	N(19)-C(15)-C(2)	121.417	C(12)-C(7)-C(8)	120.12
H(45)-C(27)-C(26)	127.021	C(16)-C(15)-C(2)	123.992	C(12)-C(7)-N(5)	118.483
H(45)-C(27)-C(23)	126.361	H(42)-C(14)-H(41)	107.882	C(8)-C(7)-N(5)	121.396
C(26)-C(27)-C(23)	106.57	H(42)-C(14)-H(40)	107.572	C(7)-N(5)-N(4)	120.166
C(31)-C(26)-C(27)	135.65	H(42)-C(14)-C(3)	111.238	C(7)-N(5)-C(1)	125.084
C(31)-C(26)-C(25)	118.848	H(41)-C(14)-H(40)	109.534	N(4)-N(5)-C(1)	109.649
C(27)-C(26)-C(25)	105.494	H(41)-C(14)-C(3)	110.977	C(13)-N(4)-N(5)	113.846
C(28)-C(25)-C(26)	123.665	H(40)-C(14)-C(3)	109.555	C(13)-N(4)-C(3)	119.521
C(28)-C(25)-O(24)	125.719	H(39)-C(13)-H(38)	109.71	N(5)-N(4)-C(3)	106.585
C(26)-C(25)-O(24)	110.61	H(39)-C(13)-H(37)	109.967	C(14)-C(3)-N(4)	118.97
C(25)-O(24)-C(23)	105.908	H(39)-C(13)-N(4)	111.563	C(14)-C(3)-C(2)	130.565
C(27)-C(23)-O(24)	111.418	H(38)-C(13)-H(37)	108.717	N(4)-C(3)-C(2)	110.46
C(27)-C(23)-C(21)	133.217	H(38)-C(13)-N(4)	108.288	C(15)-C(2)-C(3)	129.961
O(24)-C(23)-C(21)	115.208	H(37)-C(13)-N(4)	108.531	C(15)-C(2)-C(1)	122.125
C(23)-C(21)-O(22)	123.339	H(36)-C(12)-C(11)	120.83	C(3)-C(2)-C(1)	107.86
C(23)-C(21)-N(20)	114.755	H(36)-C(12)-C(7)	119.677	O(6)-C(1)-N(5)	124.099
O(22)-C(21)-N(20)	121.875	C(11)-C(12)-C(7)	119.492	O(6)-C(1)-C(2)	130.947
H(44)-N(20)-C(21)	120.923	H(35)-C(11)-C(12)	119.52	N(5)-C(1)-C(2)	104.931