Selective mercury ion recognition using methyl red (MR) based silatrane sensor

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SUPPORTING INFORMATION

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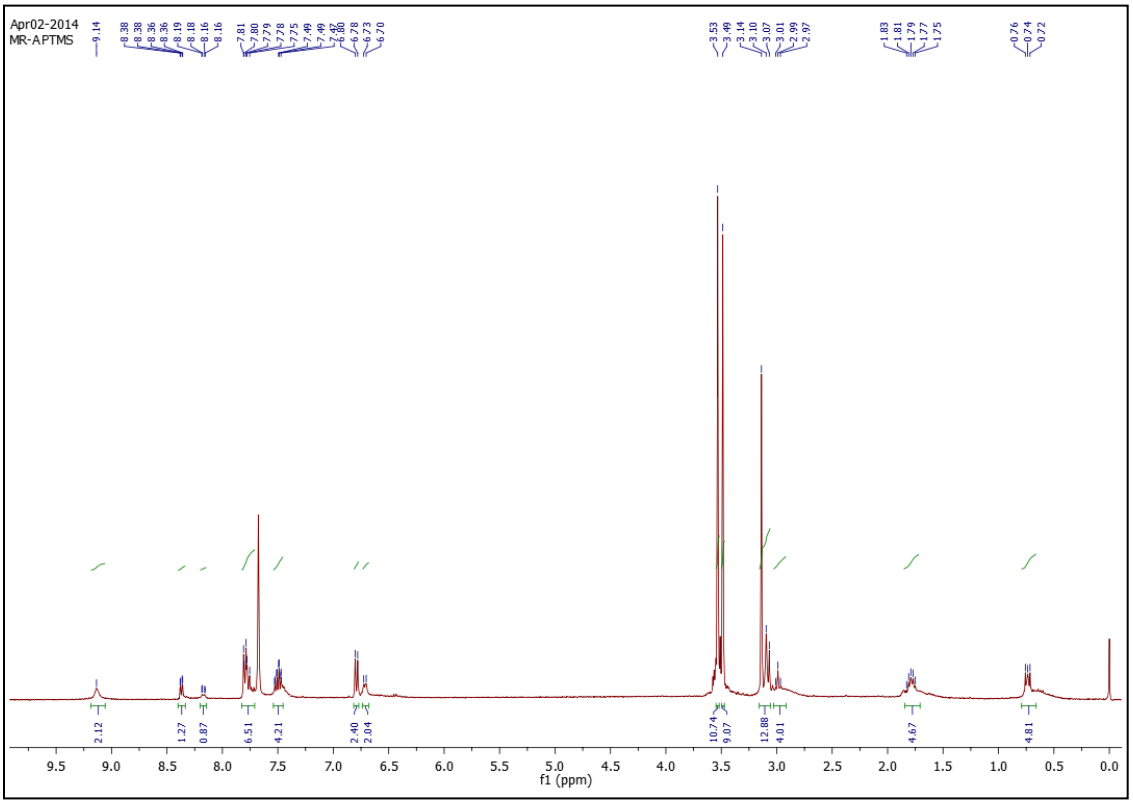

Figure S1: ^{1}H NMR spectrum of **1**

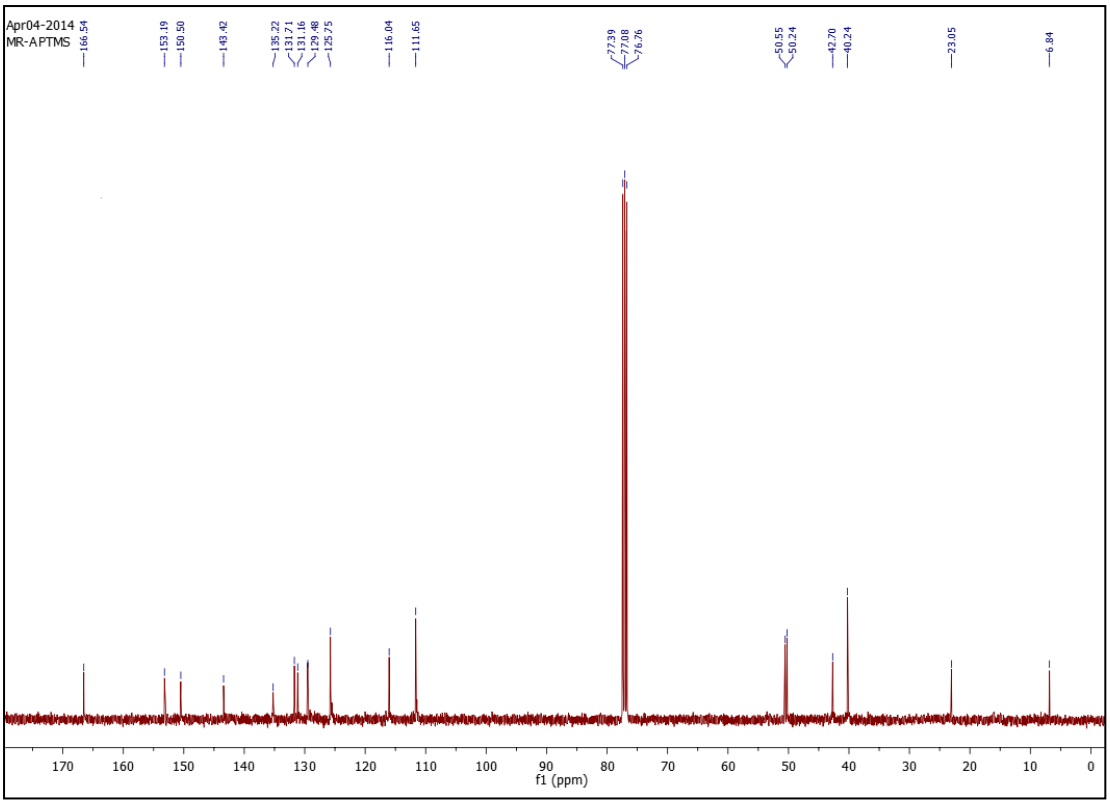

Figure S2: ^{13}C NMR spectrum of **1**

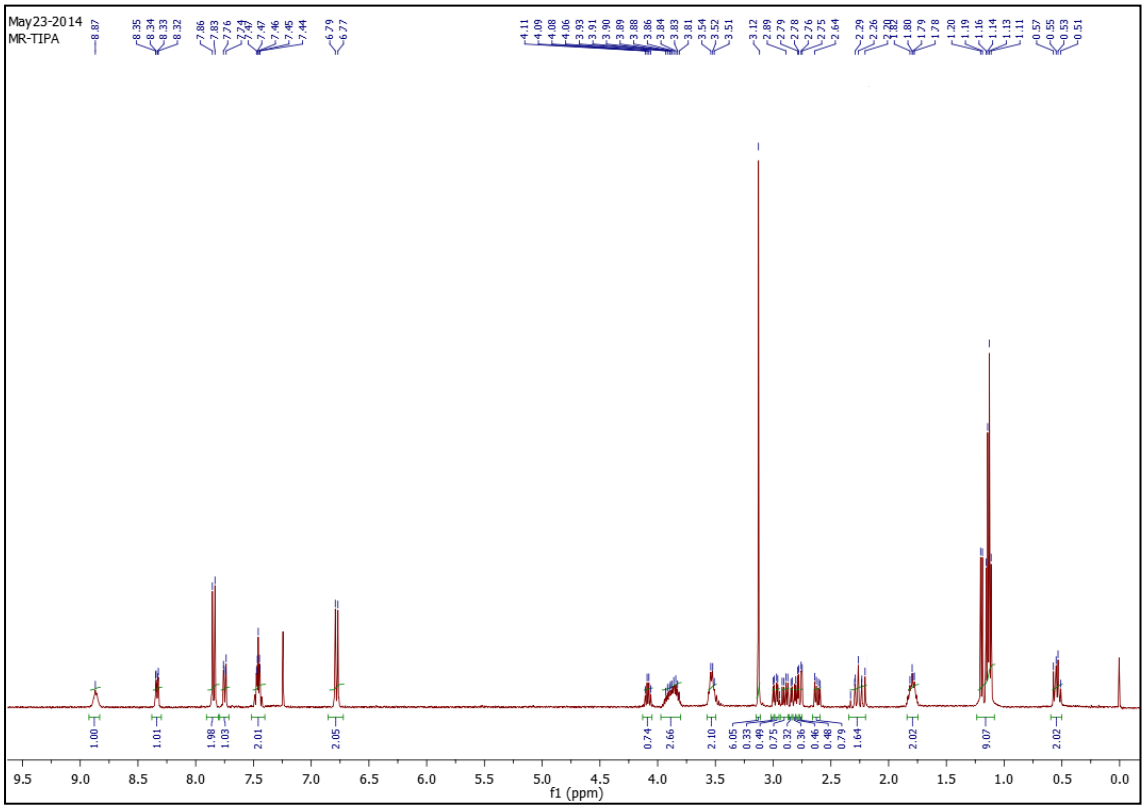

Figure S3: ^{1}H NMR spectrum of **2**

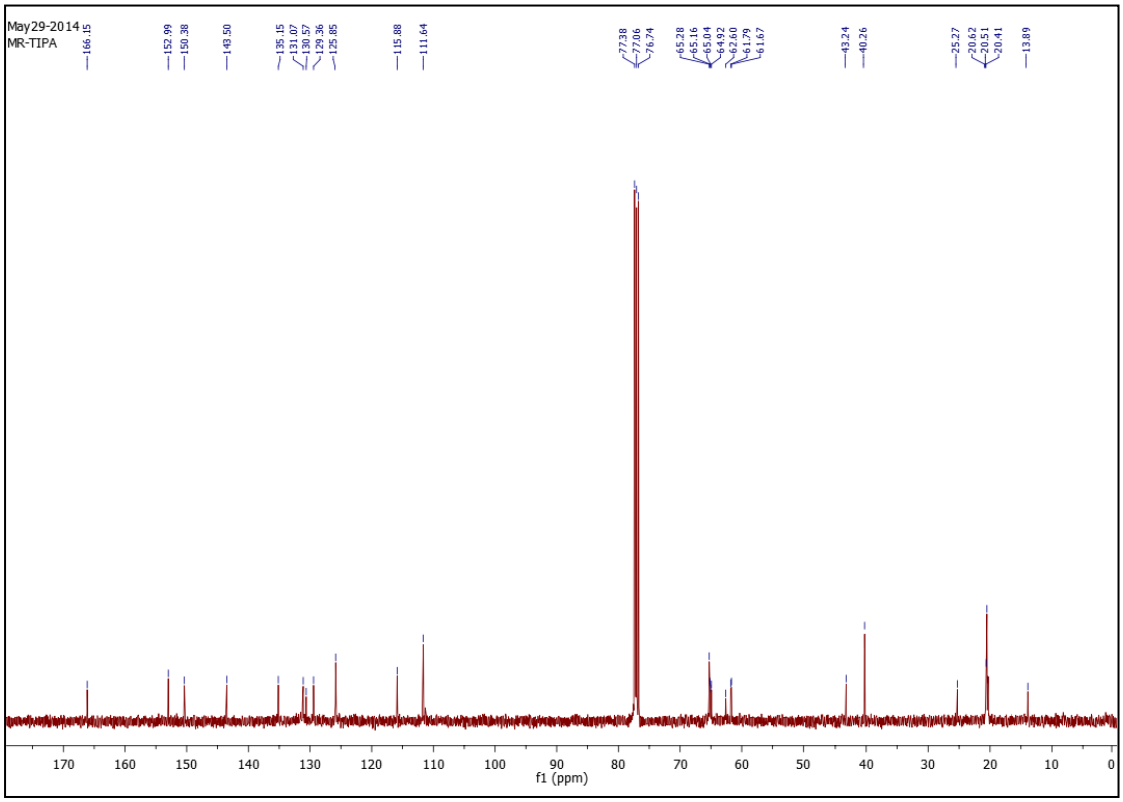

Figure S4: ^{13}C NMR spectrum of **2**

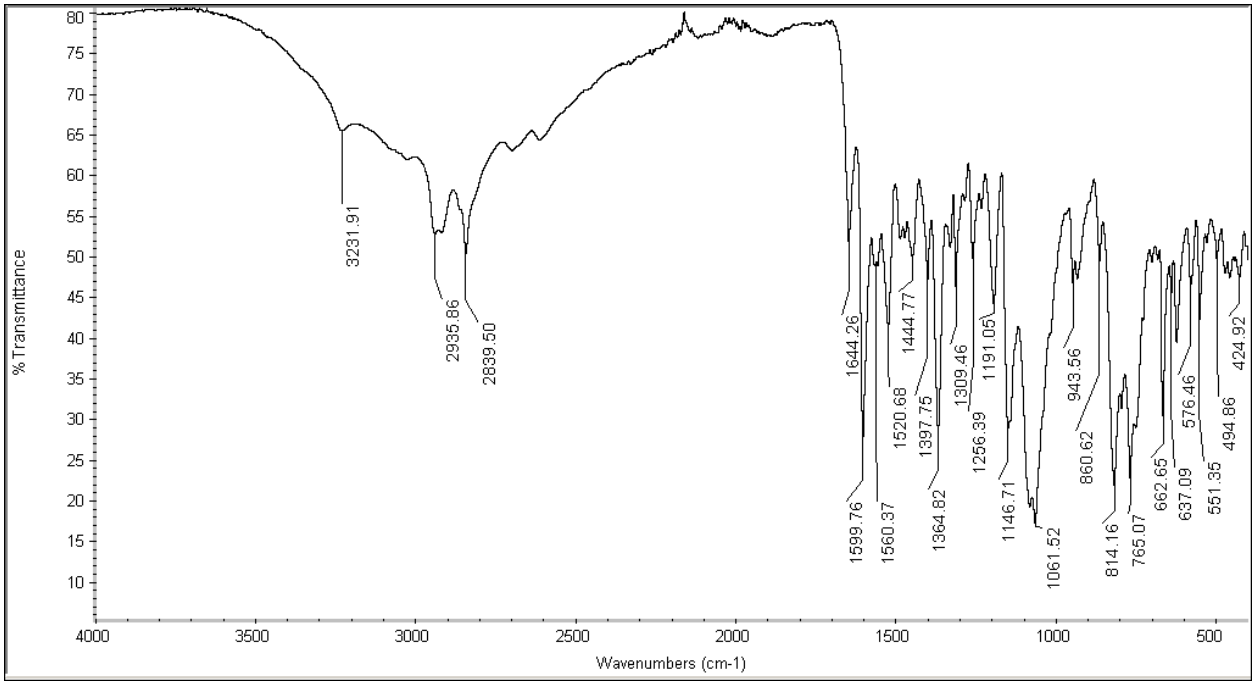

Figure S5: FTIR spectrum of **1**

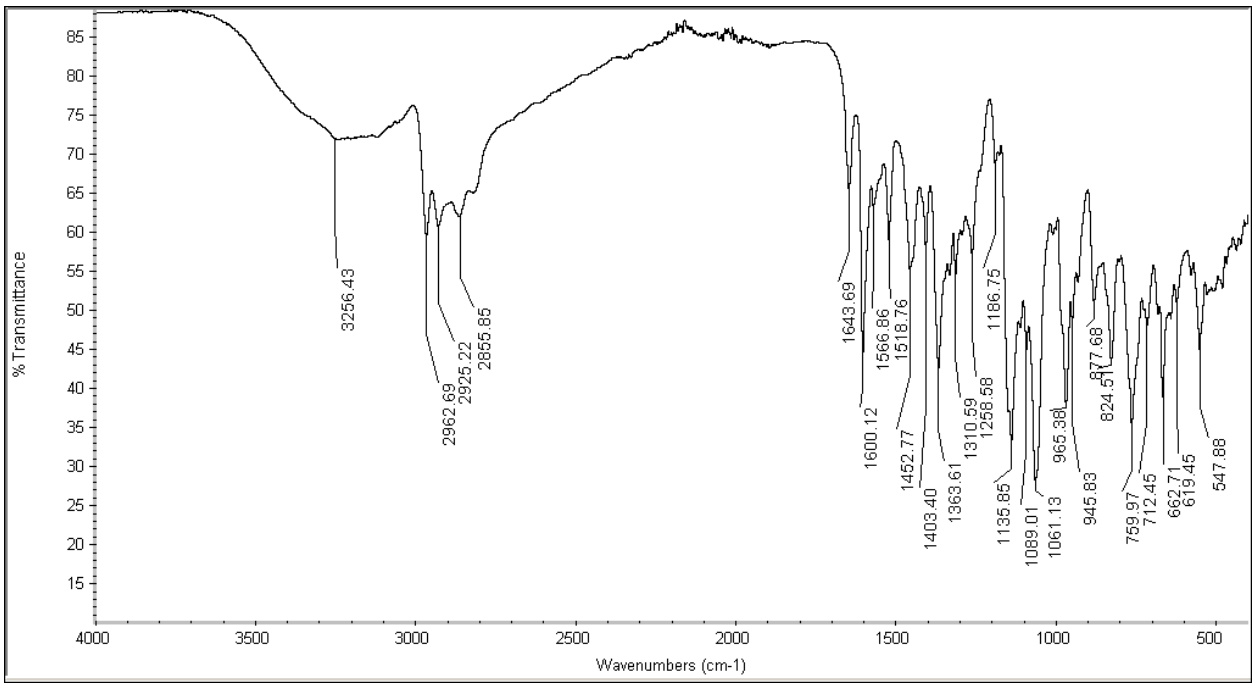

Figure S6: FTIR spectrum of **2**

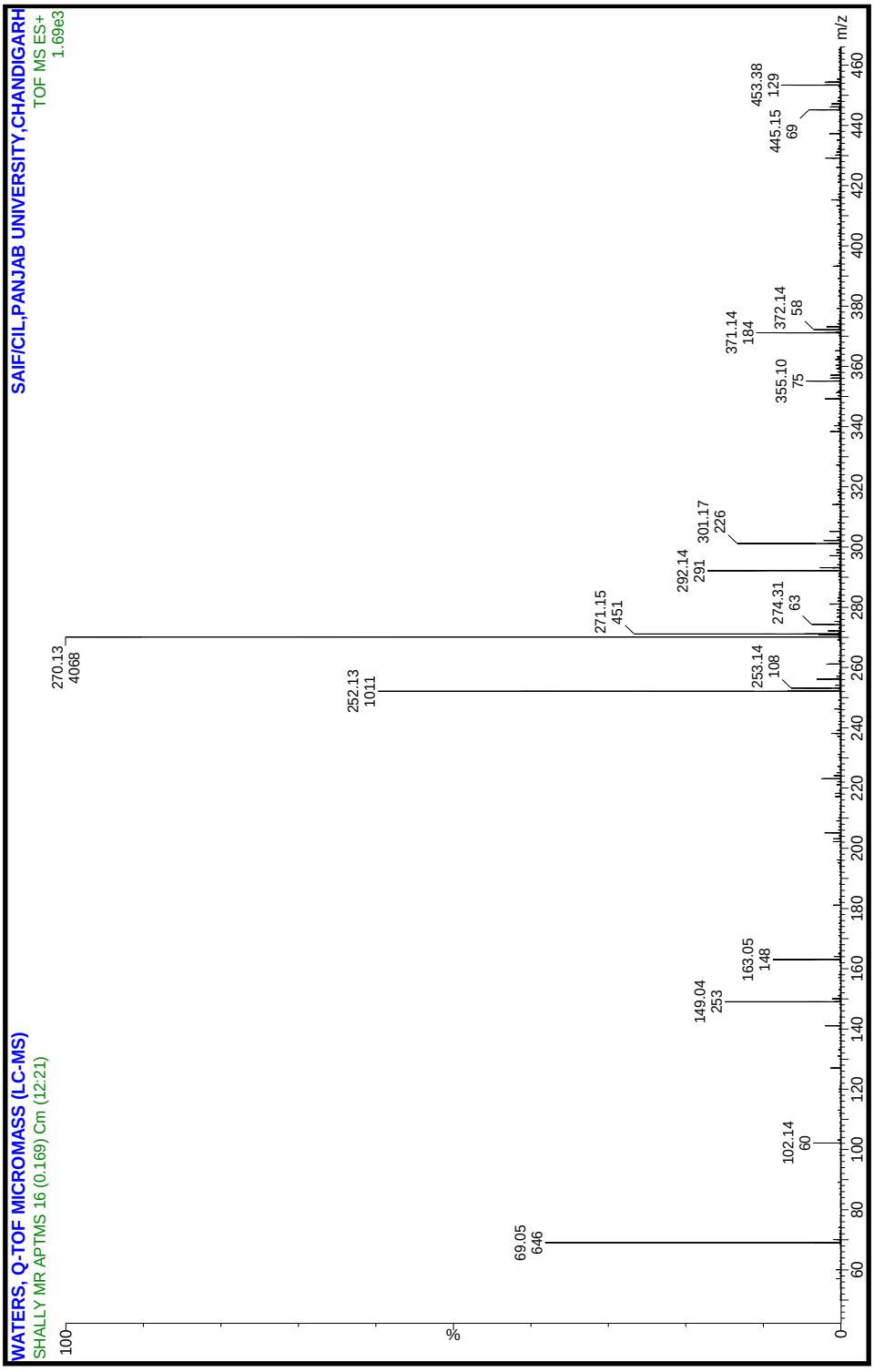

Figure S7: Mass spectrum of **1**

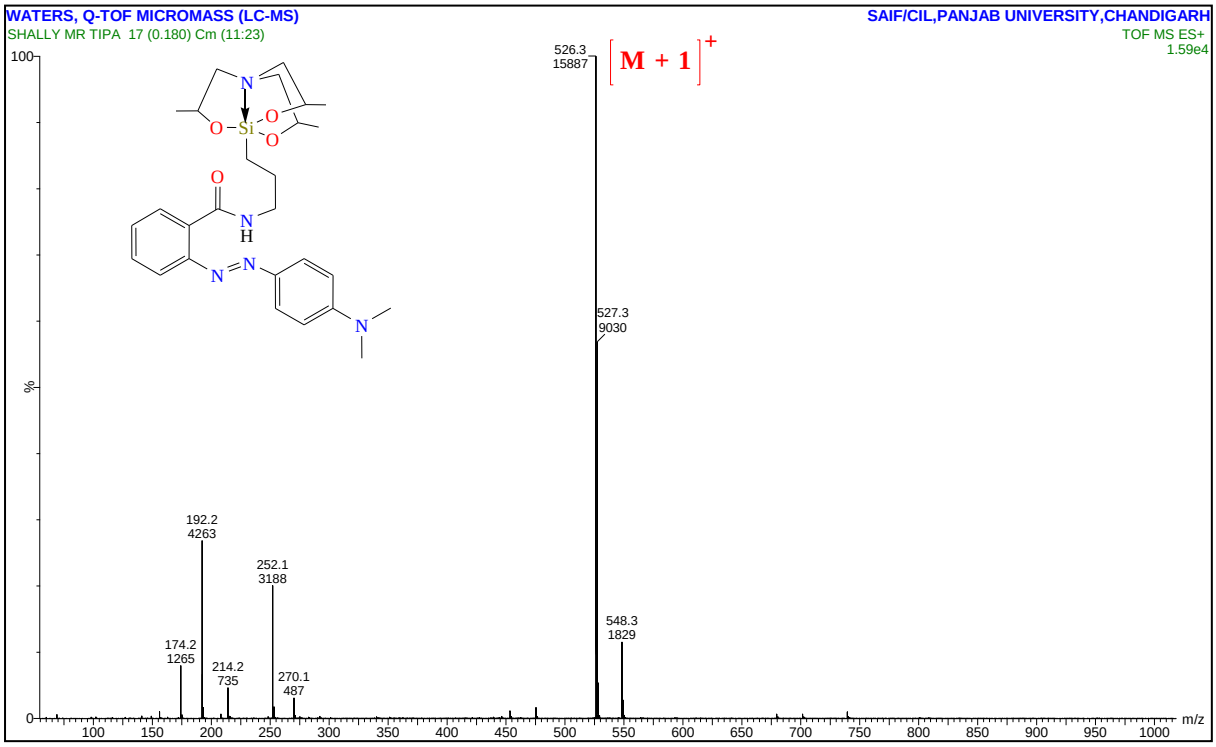

Figure S8 (a): Mass spectrum of **2**

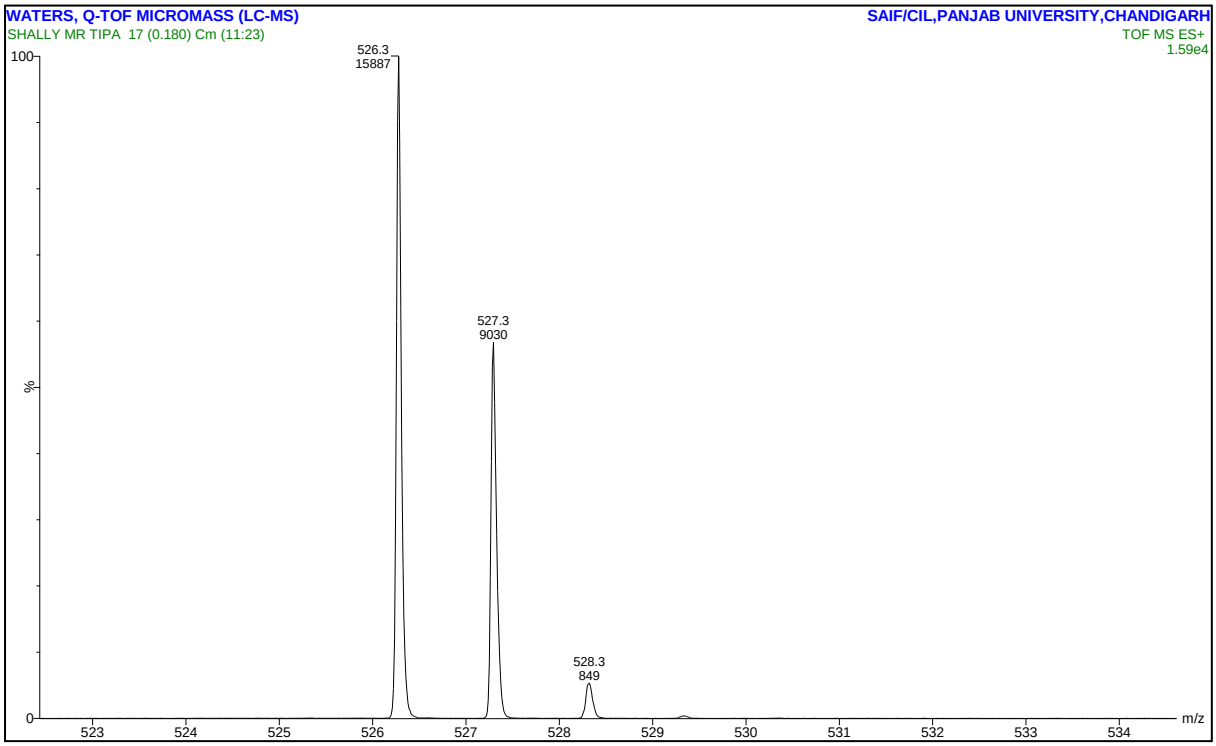

Figure S8 (b): Mass spectrum of **2**

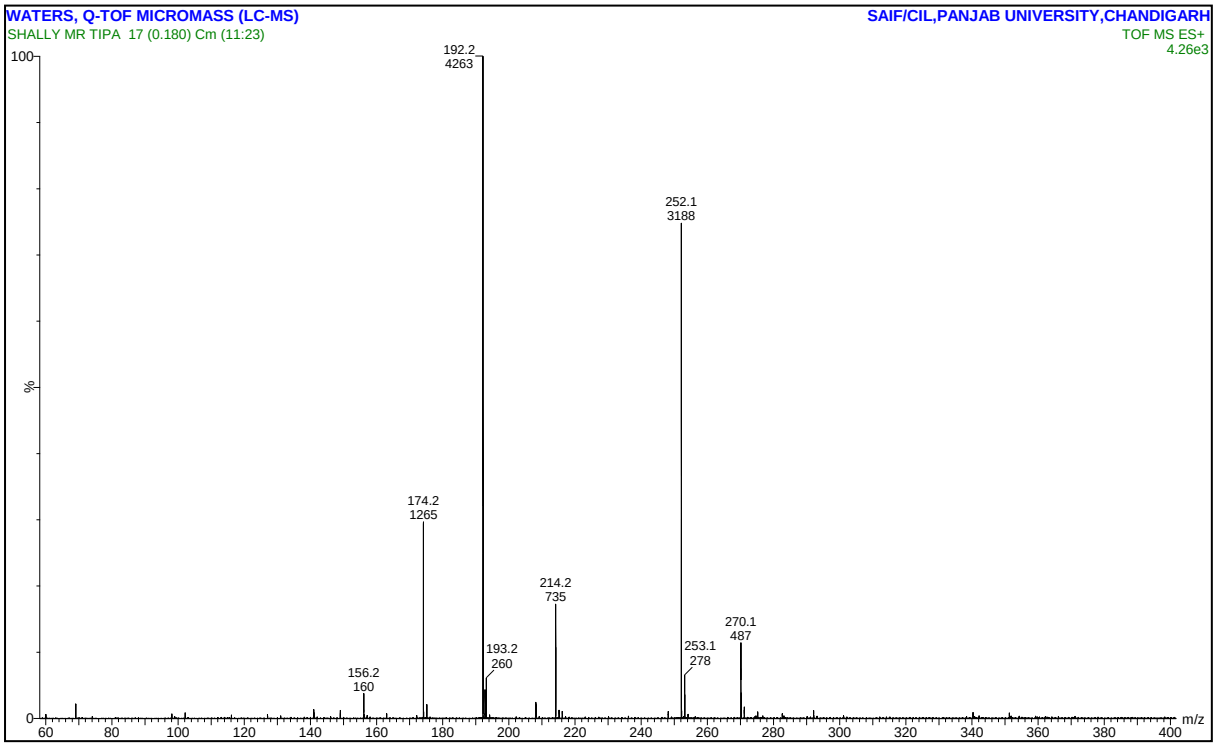

Figure S8 (c): Mass spectrum of **2**

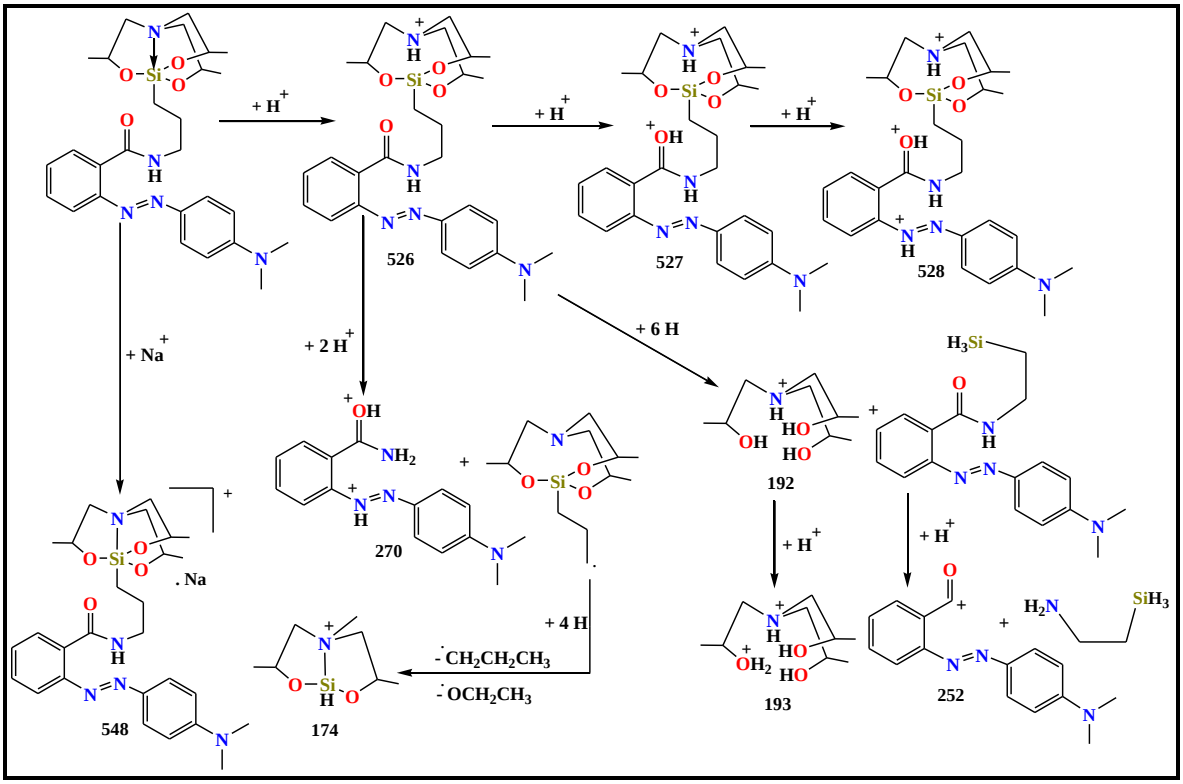

Figure S9: Proposed mass fragmentation pattern of **2**

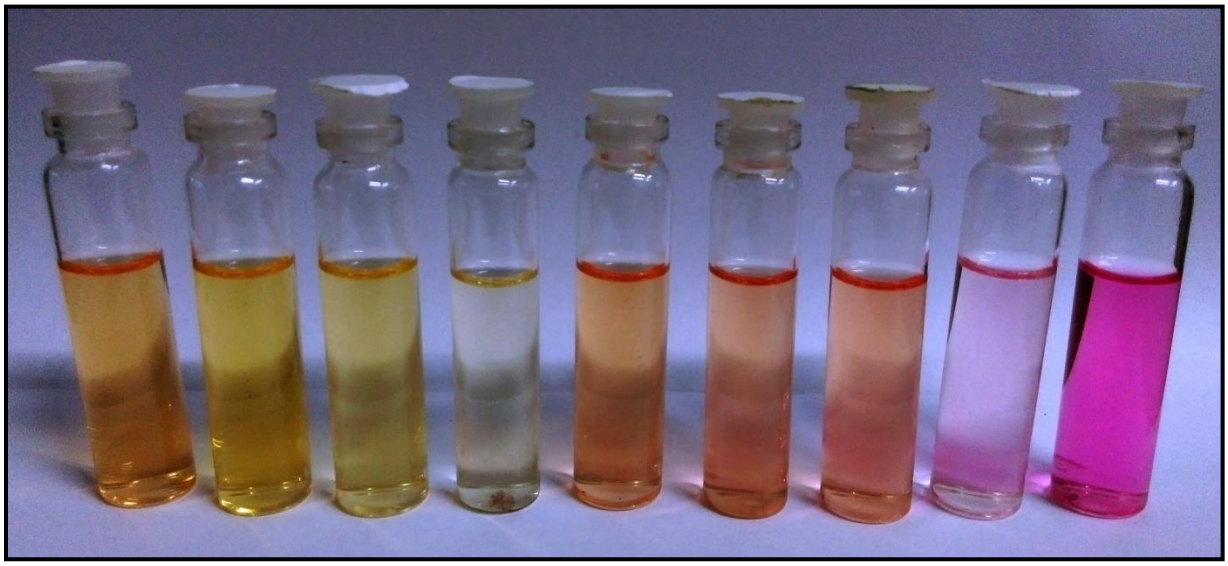

Figure S10. Illustration of gradual chromogenic change in compound **2** upon addition of Hg^{2+} ion (the vial on the extreme left shows the original color of CH_3CN solution of compound **2**)

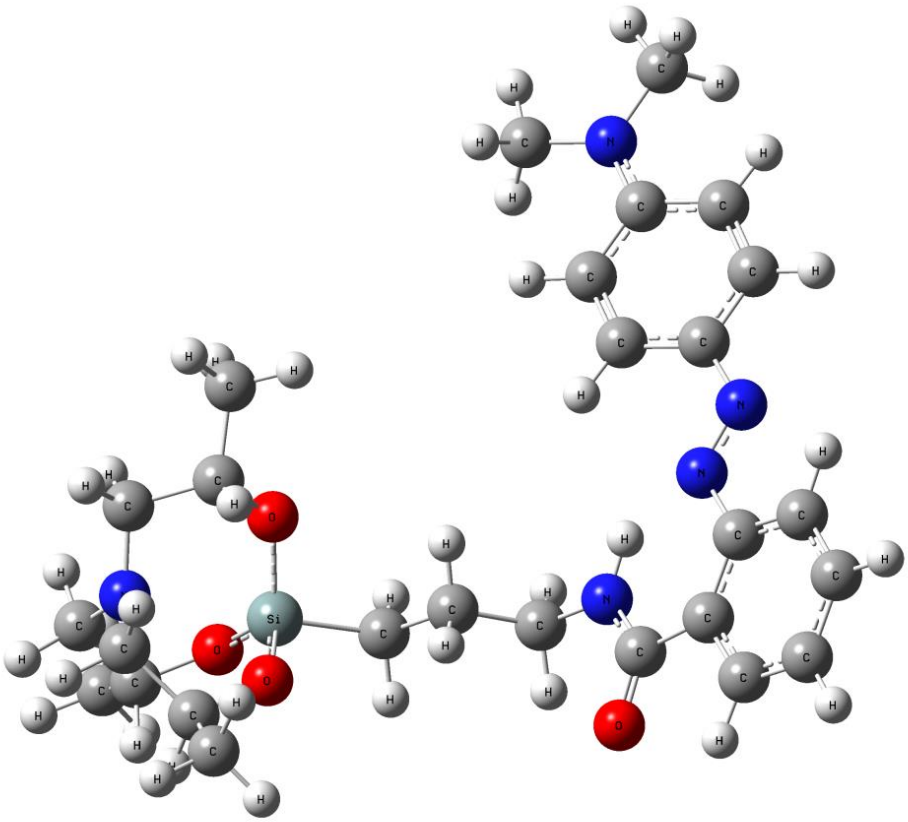

Figure S11. Plot of optimized structure of MR-APS **2**

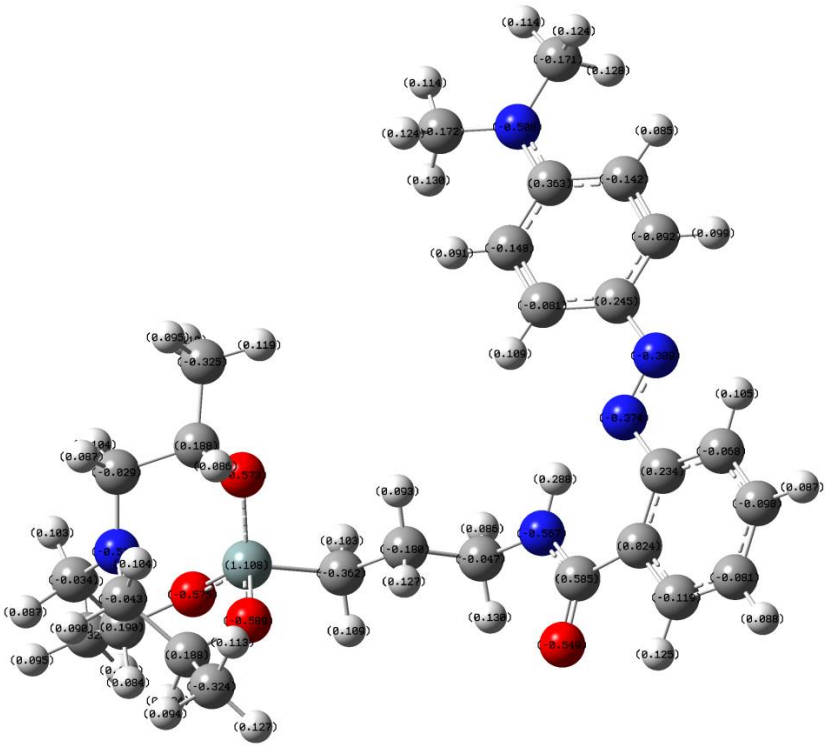

Figure S12. Plot of optimized structure of MR-APS **2** showing charge distribution

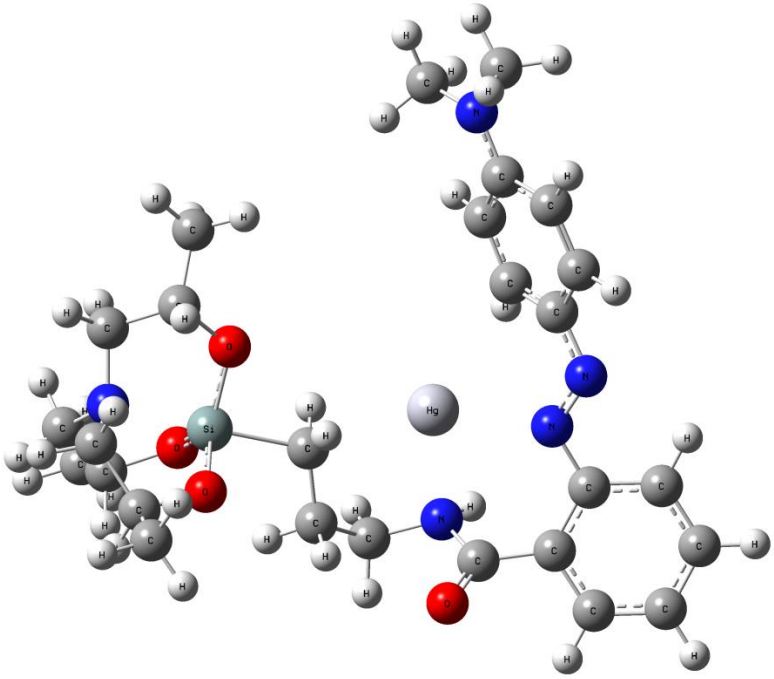

Figure S13. Plot of optimized structure of interaction complex, MR-APS-Hg^{2+} **3**

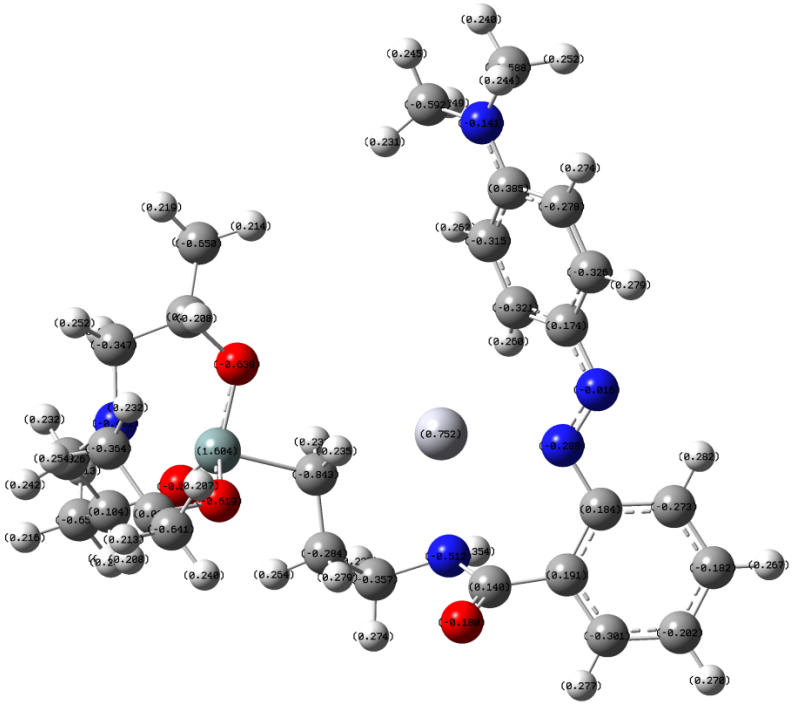

Figure S14. Plot of optimized structure of interaction complex, MR-APS-Hg^{2+} **3** showing charge distribution

Table T1. Bond lengths [Å] of **2** from X-ray Crystal structure analysis

Si1-O2	1.531(3)	**Si1-O3**	1.540(3)
Si1-O1	1.545(3)	**Si1-C10**	1.752(4)
Si1-N1	2.109(3)	**O1-C8**	1.278(5)
O2-C5	1.294(6)	**O3-C2**	1.343(5)
O4-C13	1.144(4)	**N1-C3**	1.363(5)
N1-C4	1.366(5)	**N1-C7**	1.367(5)
N2-C13	1.243(5)	**N2-C12**	1.360(5)
N2-H2	0.86	**N3-N4**	1.184(4)
N3-C19	1.335(5)	**N4-C20**	1.302(5)
N5-C23	1.276(5)	**N5-C26**	1.352(5)
N5-C27	1.358(5)	**C1-C2**	1.400(6)
C1-H1B	0.96	**C1-H1C**	0.96
C1-H1A	0.96	**C2-C3**	1.374(6)
C2-H2A	0.98	**C3-H3B**	0.97
C3-H3A	0.97	**C4-C5**	1.301(7)
C4-H4B	0.97	**C4-H4A**	0.97
C5-C6	1.347(6)	**C5-H5**	0.98

C6-H6B	0.96	**C6-H6C**	0.96
C6-H6A	0.96	**C7-C8**	1.279(6)
C7-H7B	0.97	**C7-H7A**	0.97
C8-C9	1.346(6)	**C8-H8**	0.98
C9-H9B	0.96	**C9-H9C**	0.96
C9-H9A	0.96	**C10-C11**	1.423(5)
C10-H10A	0.97	**C10-H10B**	0.97
C11-C12	1.420(5)	**C11-H11B**	0.97
C11-H11A	0.97	**C12-H12B**	0.97
C12-H12A	0.97	**C13-C14**	1.406(6)
C14-C15	1.300(5)	**C14-C19**	1.303(5)
C15-C16	1.284(6)	**C15-H13**	0.93
C16-C17	1.279(7)	**C16-H14**	0.93
C17-C18	1.282(6)	**C17-H15**	0.93
C18-C19	1.294(6)	**C18-H16**	0.93
C20-C25	1.283(5)	**C20-C21**	1.299(5)
C21-C22	1.286(5)	**C21-H17**	0.93
C22-C23	1.295(5)	**C22-H18**	0.93
C23-C24	1.320(5)	**C24-C25**	1.282(5)
C24-H19	0.93	**C25-H20**	0.93
C26-H22B	0.96	**C26-H22A**	0.96
C26-H22C	0.96	**C27-H21A**	0.96
C27-H21C	0.96	**C27-H21B**	0.96

Table T2. Bond angles [°] of **2** from X-ray Crystal structure analysis

O2-Si1-O3	118.06(16)	**O2-Si1-C10**	117.67(16)
O3-Si1-O1	117.25(16)	**O1-Si1-C10**	100.05(17)
O3-Si1-C10	98.73(17)	**O3-Si1-N1**	97.84(16)
O2-Si1-N1	81.13(14)	**C10-Si1-N1**	81.04(14)
O1-Si1-N1	81.19(13)	**C5-O2-Si1**	178.74(16)
C8-O1-Si1	124.4(3)	**C3-N1-C4**	124.9(3)
C2-O3-Si1	122.6(3)	**C4-N1-C7**	114.1(4)
C3-N1-C7	115.3(4)	**C4-N1-Si1**	114.3(4)
C3-N1-Si1	104.3(3)	**C13-N2-C12**	103.5(3)
C7-N1-Si1	103.3(3)	**C12-N2-H2**	122.0(4)
C13-N2-H2	119.0	**N3-N4-C20**	119.0
N4-N3-C19	113.7(4)	**C23-N5-C27**	116.4(3)
C23-N5-C26	122.1(4)	**C2-C1-H1B**	121.0(4)
C26-N5-C27	116.7(4)	**H1B-C1-H1C**	109.5
C2-C1-H1C	109.5	**H1B-C1-H1A**	109.5
C2-C1-H1A	109.5	**O3-C2-C3**	109.5

H1C-C1-H1A	109.5	**C3-C2-C1**	109.2(4)
O3-C2-C1	109.7(4)	**C3-C2-H2A**	114.9(5)
O3-C2-H2A	107.6	**N1-C3-C2**	107.6
C1-C2-H2A	107.6	**C2-C3-H3B**	109.7(4)
N1-C3-H3B	109.7	**C2-C3-H3A**	109.7
N1-C3-H3A	109.7	**C5-C4-N1**	109.7
H3B-C3-H3A	108.2	**N1-C4-H4B**	112.3(4)
C5-C4-H4B	109.1	**N1-C4-H4A**	109.1
C5-C4-H4A	109.1	**O2-C5-C4**	109.1
H4B-C4-H4A	107.9	**C4-C5-C6**	115.9(5)
O2-C5-C6	116.7(5)	**C4-C5-H5**	121.7(6)
O2-C5-H5	98.0	**C5-C6-H6B**	98.0
C6-C5-H5	98.0	**H6B-C6-H6C**	109.5
C5-C6-H6C	109.5	**H6B-C6-H6A**	109.5
C5-C6-H6A	109.5	**C8-C7-N1**	109.5
H6C-C6-H6A	109.5	**N1-C7-H7B**	112.4(4)
C8-C7-H7B	109.1	**N1-C7-H7A**	109.1
C8-C7-H7A	109.1	**O1-C8-C7**	109.1
H7B-C7-H7A	107.9	**C7-C8-C9**	118.4(5)
O1-C8-C9	116.8(5)	**C7-C8-H8**	124.6(5)
O1-C8-H8	91.7	**C8-C9-H9B**	91.7
C9-C8-H8	91.7	**H9B-C9-H9C**	109.5
C8-C9-H9C	109.5	**H9B-C9-H9A**	109.5
C8-C9-H9A	109.5	**C11-C10-Si1**	109.5
H9C-C9-H9A	109.5	**Si1-C10-H10A**	114.8(3)
C11-C10-H10A	108.6	**Si1-C10-H10B**	108.6
C11-C10-H10B	108.6	**C12-C11-C10**	108.6
H10A-C10-H10B	107.5	**C10-C11-H11B**	113.8(3)
C12-C11-H11B	108.8	**C10-C11-H11A**	108.8
C12-C11-H11A	108.8	**N2-C12-C11**	108.8
H11B-C11-H11A	107.7	**C11-C12-H12B**	113.1(3)
N2-C12-H12B	109.0	**C11-C12-H12A**	109.0
N2-C12-H12A	109.0	**O4-C13-N2**	109.0
H12B-C12-H12A	107.8	**N2-C13-C14**	121.6(4)
O4-C13-C14	119.9(4)	**C15-C14-C13**	118.5(4)
C15-C14-C19	118.3(4)	**C16-C15-C14**	114.2(4)
C19-C14-C13	127.5(4)	**C14-C15-H13**	121.1(5)
C16-C15-H13	119.5	**C17-C16-H14**	119.5
C17-C16-C15	120.4(5)	**C16-C17-C18**	119.8
C15-C16-H14	119.8	**C18-C17-H15**	119.4(5)

C16-C17-H15	120.3	**C17-C18-H16**	120.3
C17-C18-C19	121.2(5)	**C18-C19-C14**	119.4
C19-C18-H16	119.4	**C14-C19-N3**	119.6(4)
C18-C19-N3	121.3(4)	**C25-C20-N4**	119.1(4)
C25-C20-C21	118.6(4)	**C22-C21-C20**	126.5(4)
C21-C20-N4	114.9(4)	**C20-C21-H17**	121.1(4)
C22-C21-H17	119.4	**C21-C22-H18**	119.4
C21-C22-C23	121.0(4)	**N5-C23-C22**	119.5
C23-C22-H18	119.5	**C22-C23-C24**	122.0(4)
N5-C23-C24	120.8(4)	**C25-C24-H19**	117.2(4)
C25-C24-C23	121.2(4)	**C24-C25-C20**	119.4
C23-C24-H19	119.4	**C20-C25-H20**	120.8(4)
C24-C25-H20	119.6	**N5-C26-H22A**	119.6
N5-C26-H22B	109.5	**N5-C26-H22C**	109.5
H22B-C26-H22A	109.5	**H22A-C26-H22C**	109.5
H22B-C26-H22C	109.5	**N5-C27-H21C**	109.5
N5-C27-H21A	109.5	**N5-C27-H21B**	109.5
H21A-C27-H21C	109.5	**H21C-C27-H21B**	109.5
H21A-C27-H21B	109.5		