

First report of X-ray characterized Organosilatrane based receptor for electrochemical analysis of Al³⁺ ions

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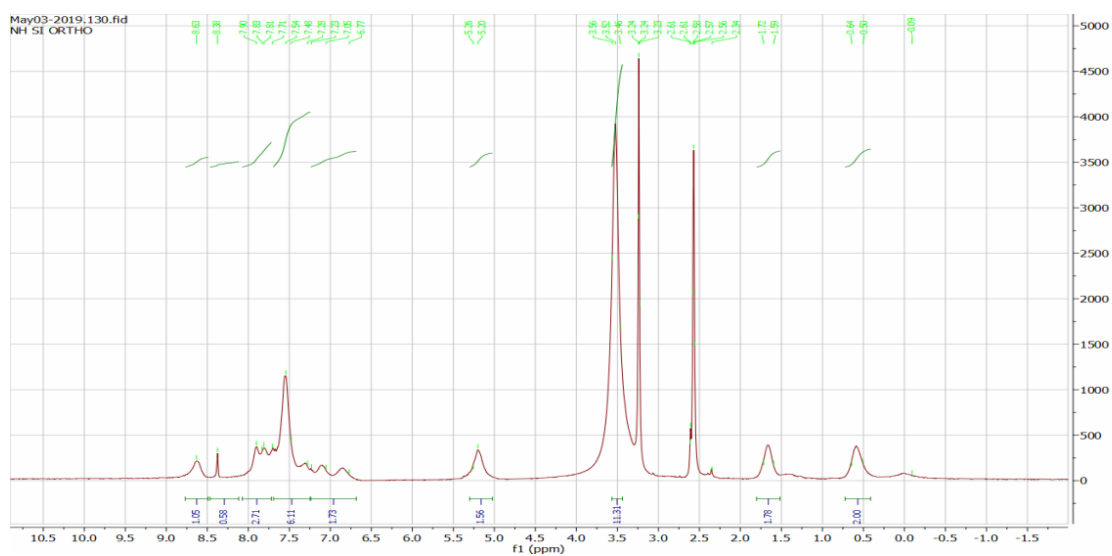
Panjab University, Chandigarh, India

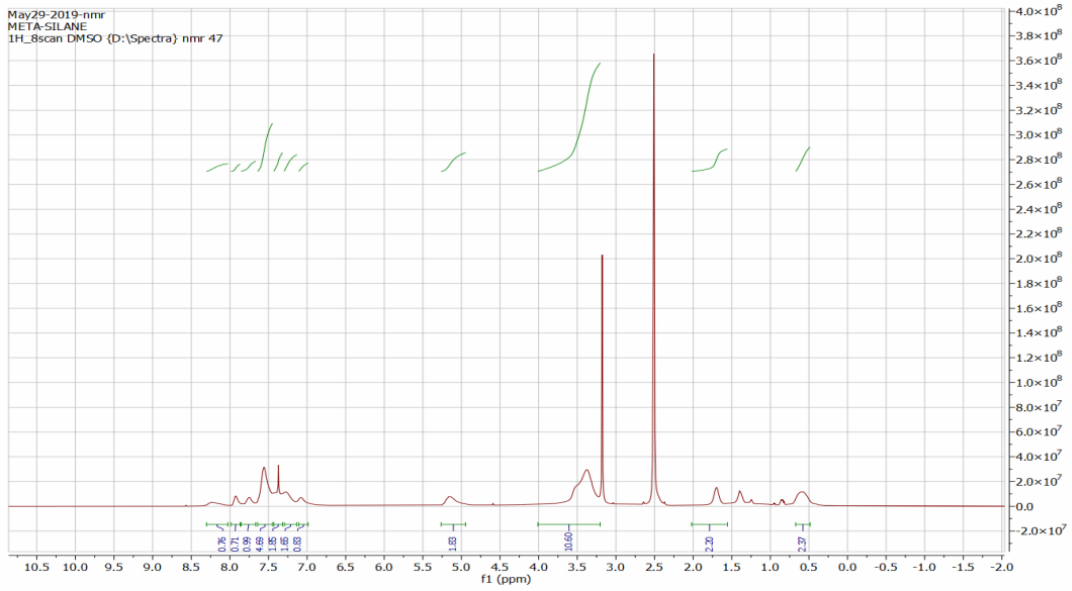
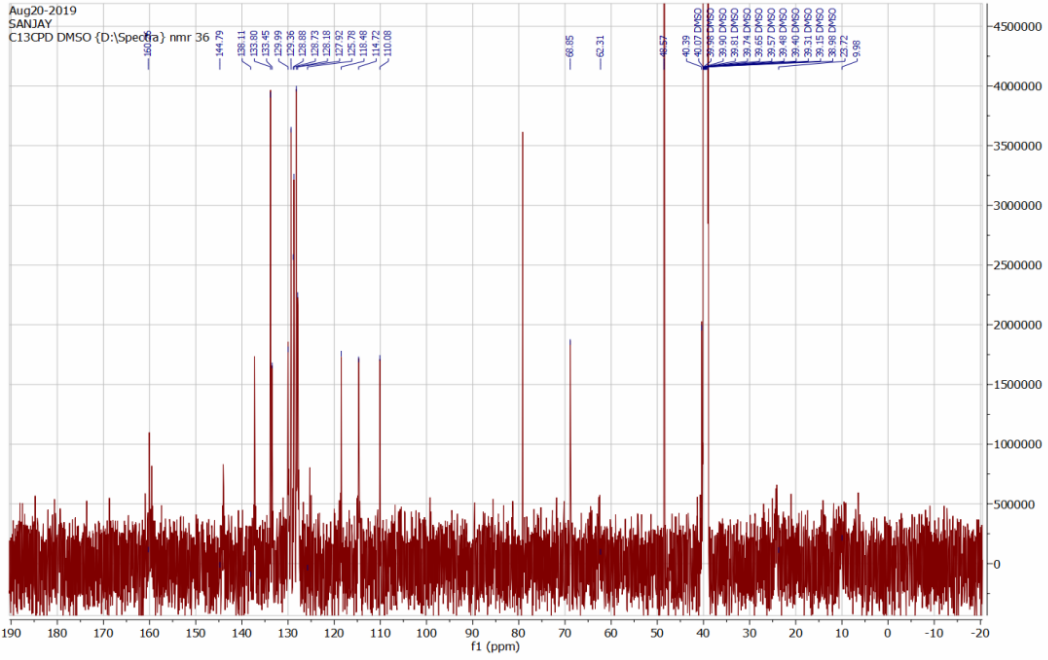
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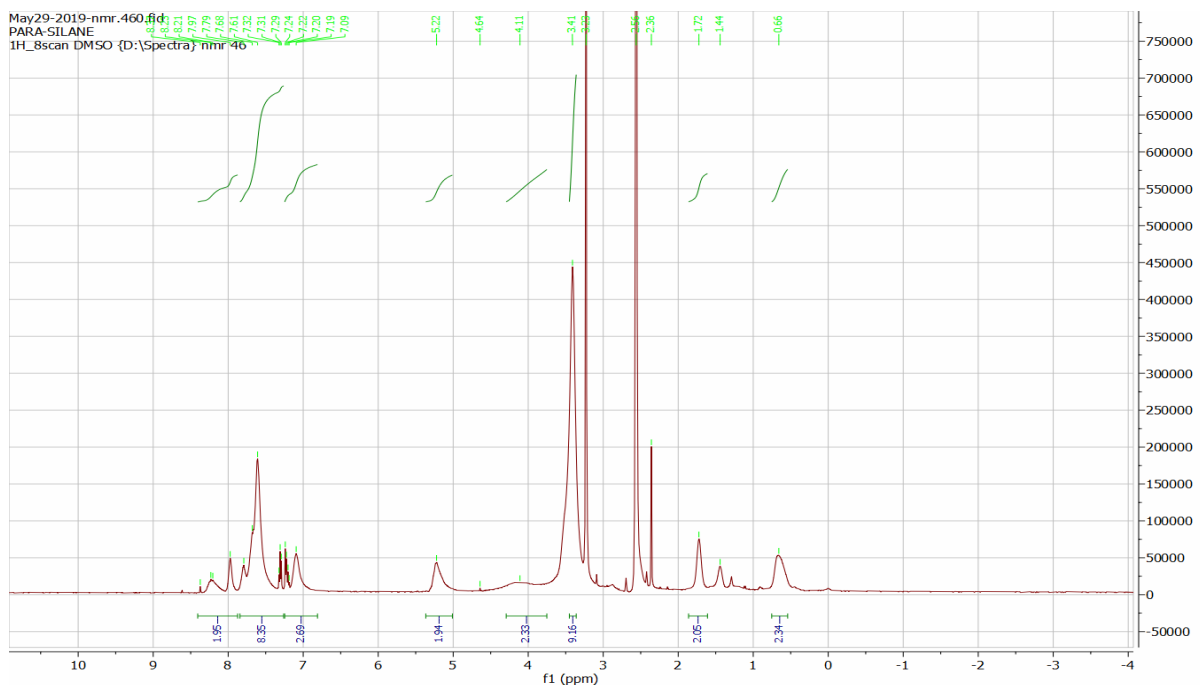
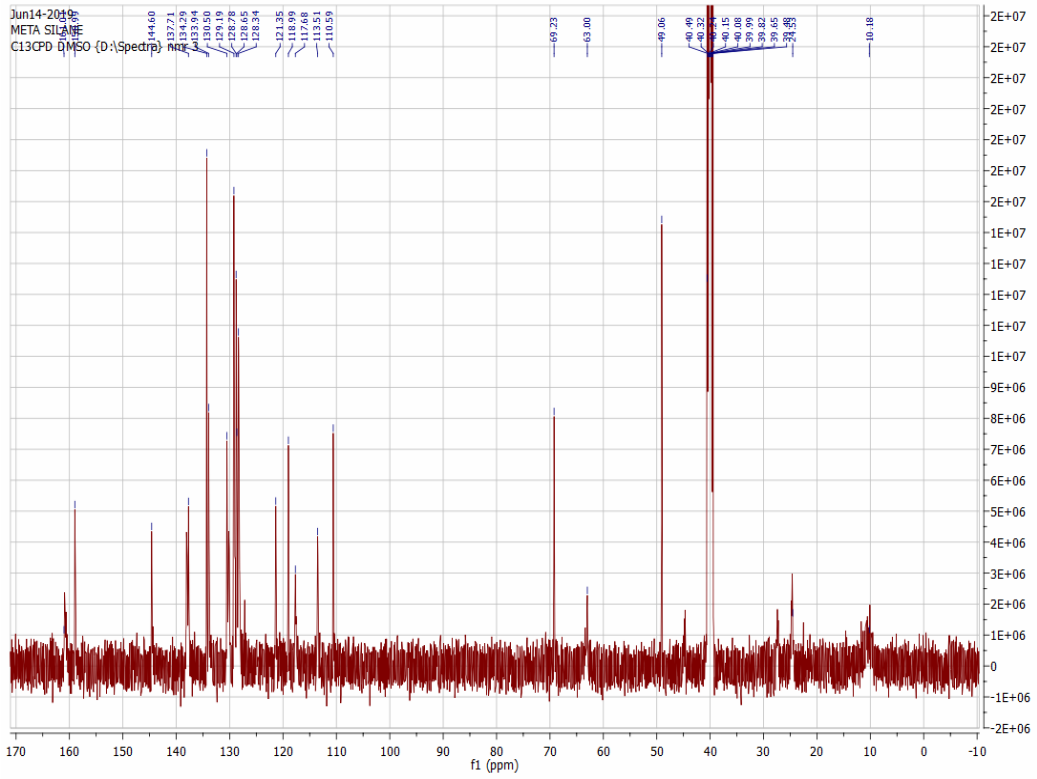
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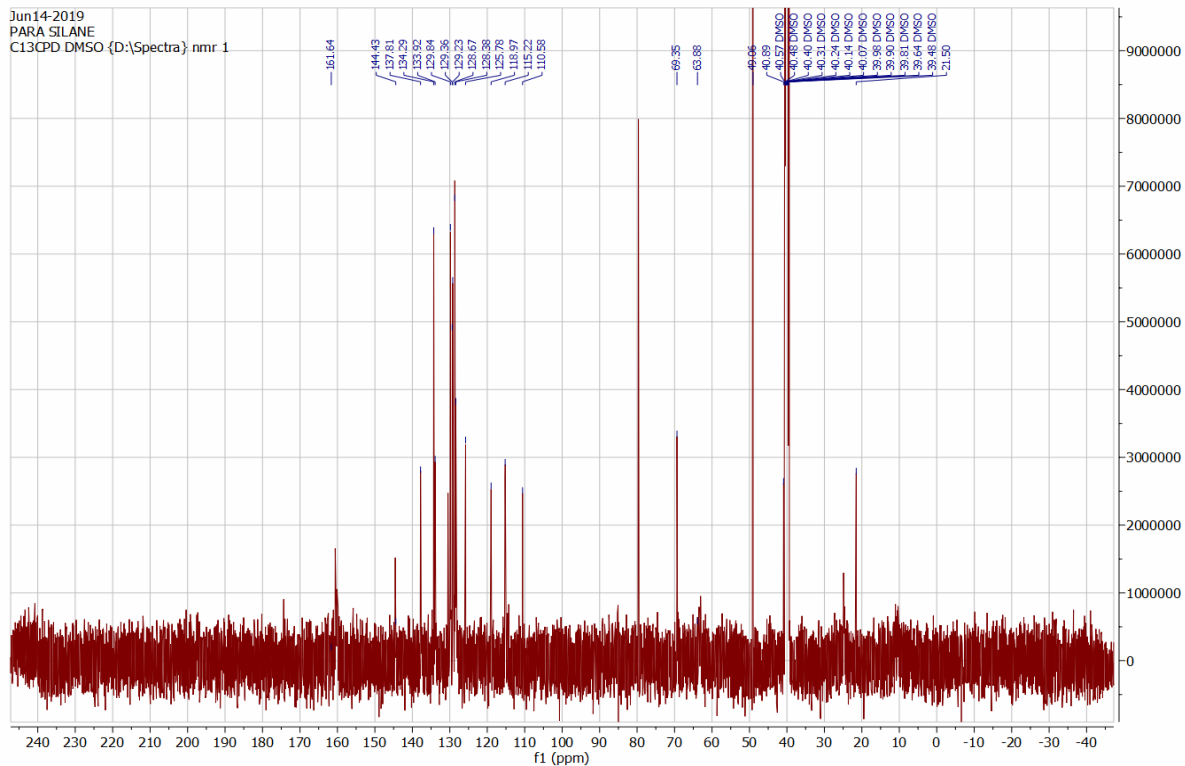
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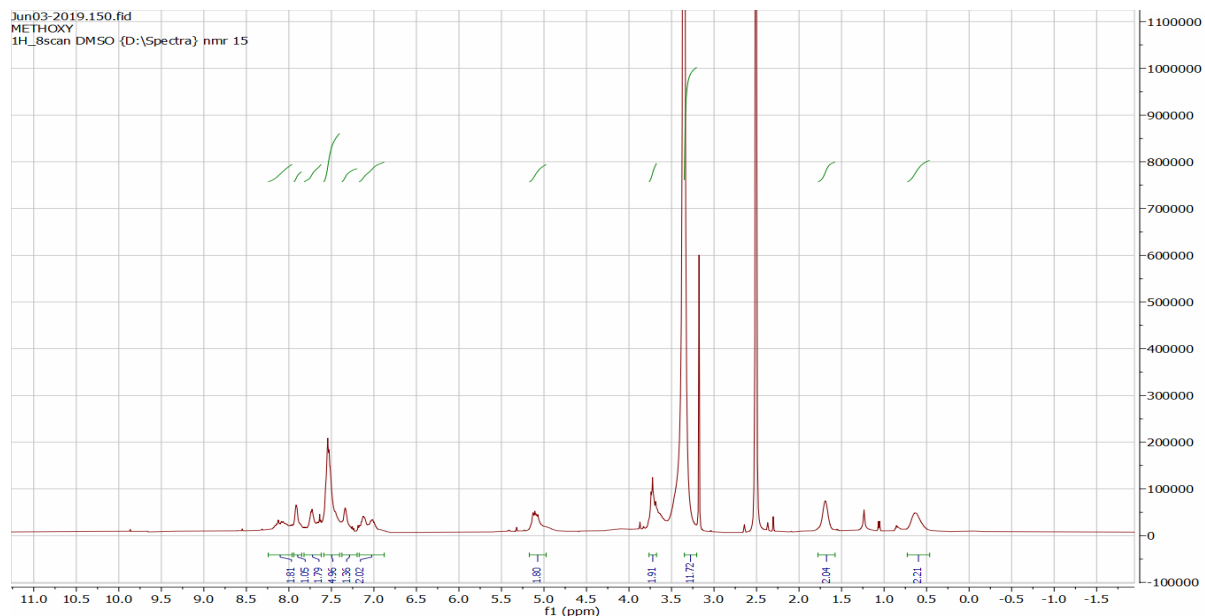


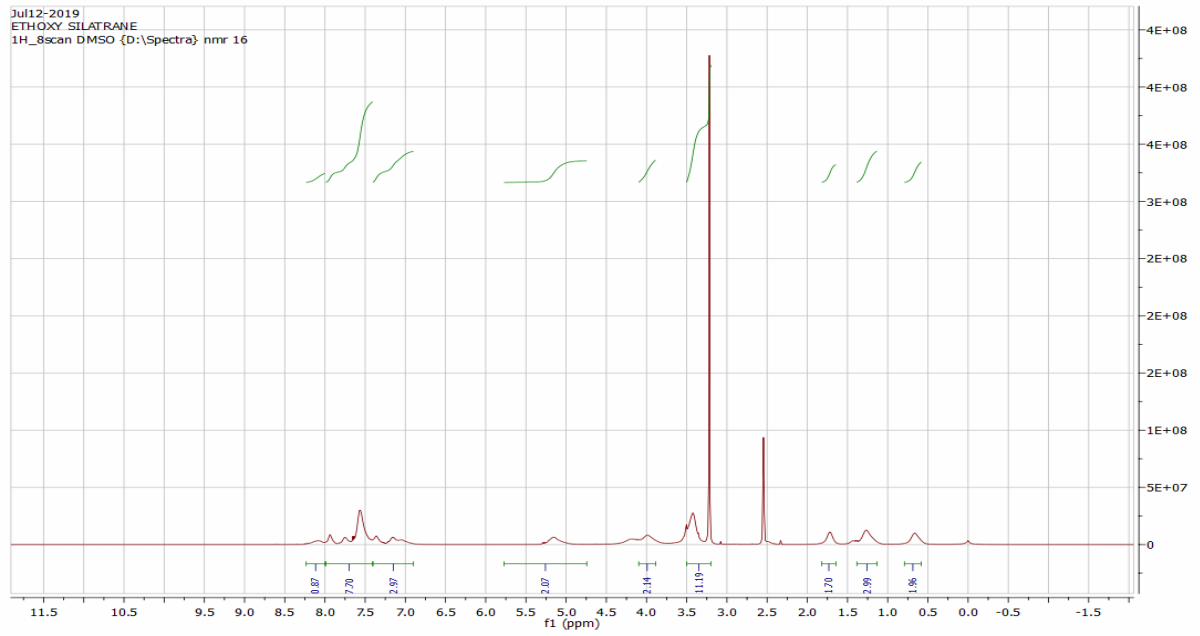
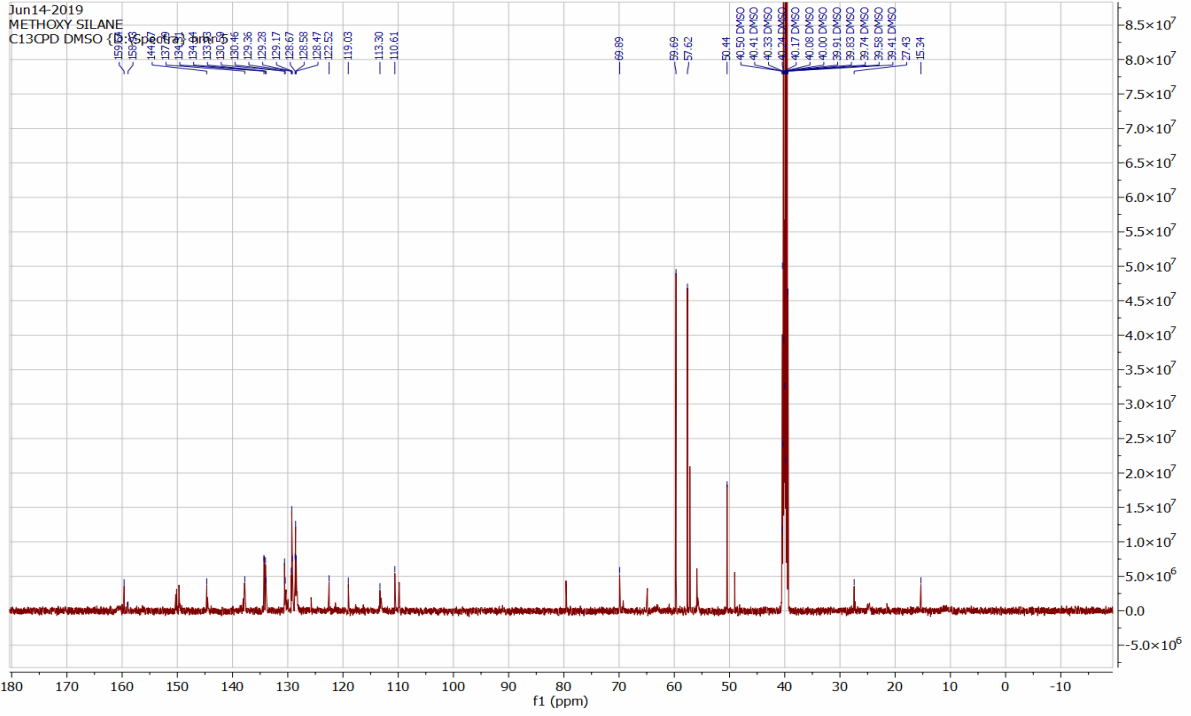


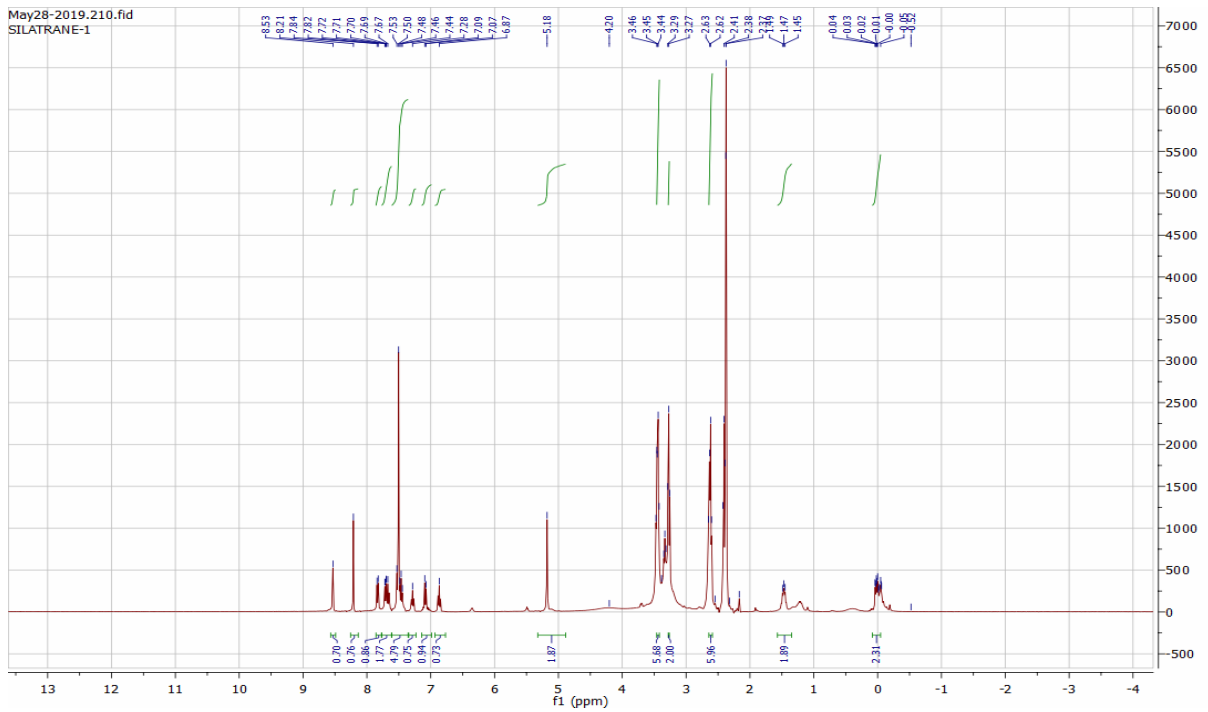
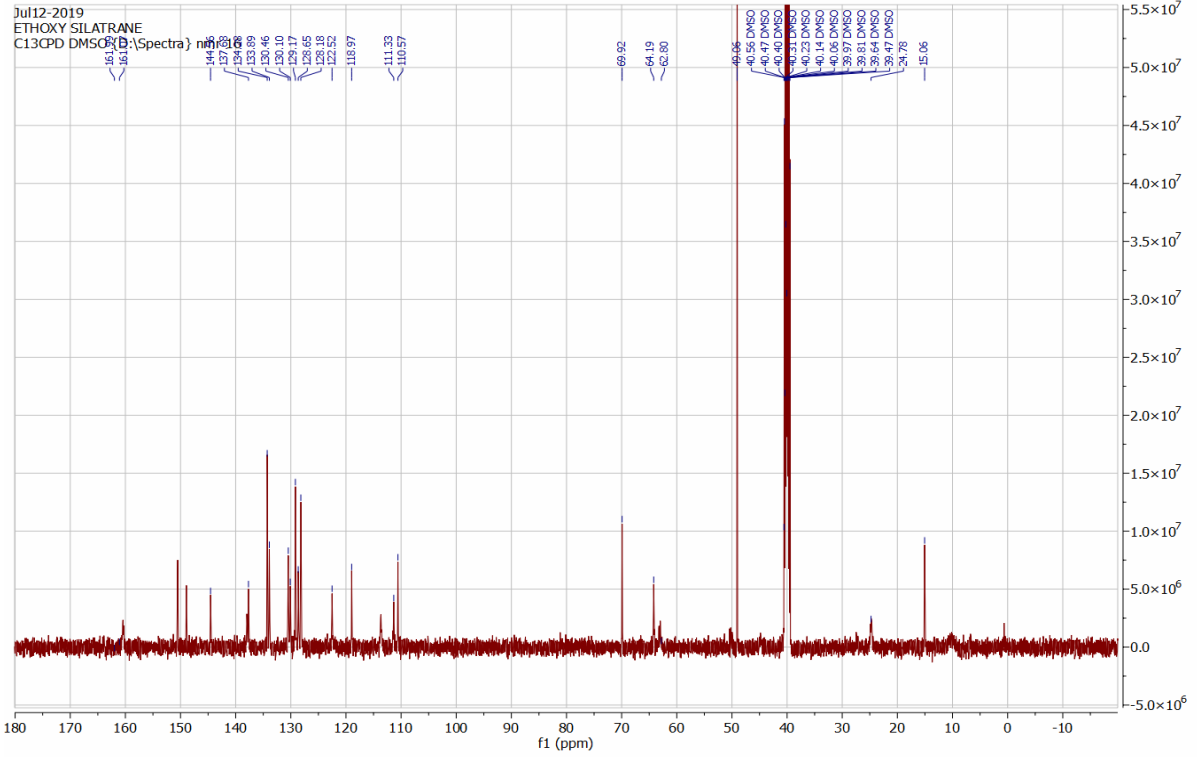
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 C13CPD DMSO {D:\Spectra} nmr 1

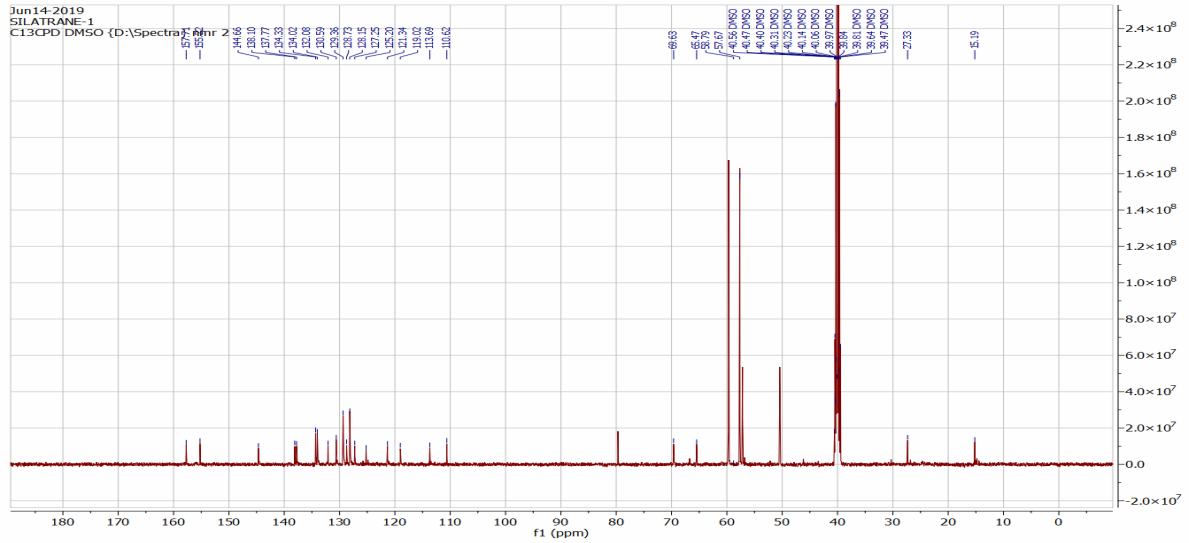


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 METHOXY
 1H_8scan DMSO {D:\Spectra} nmr 15







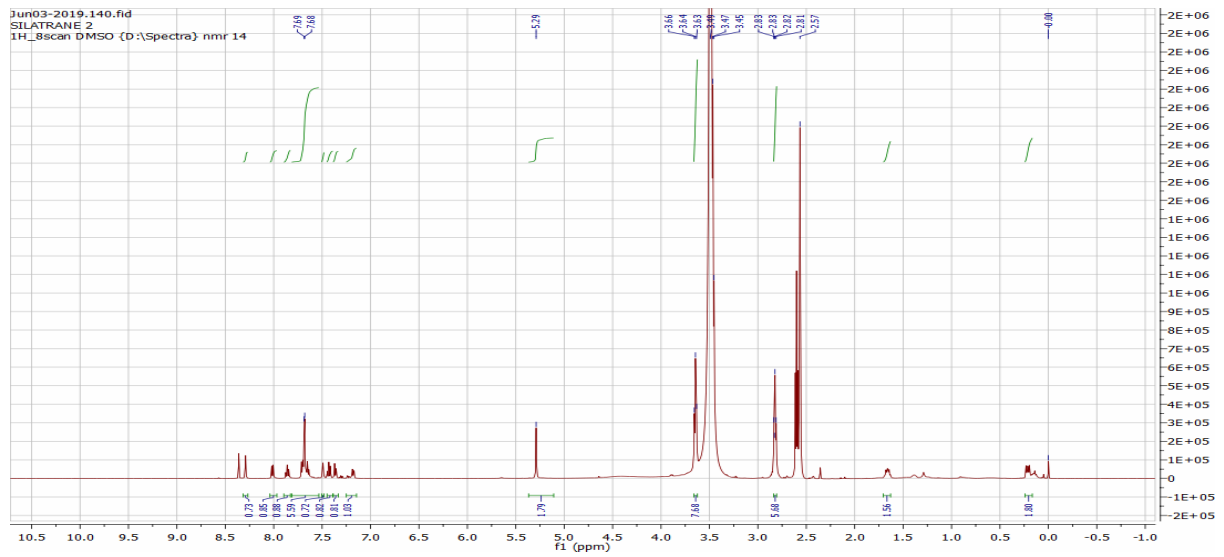
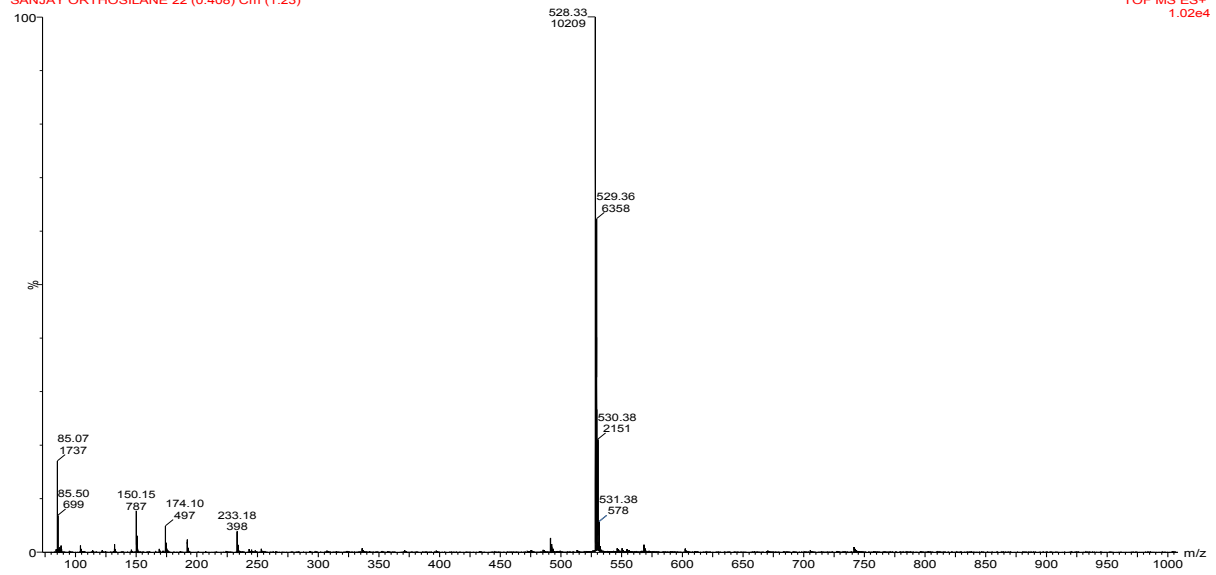


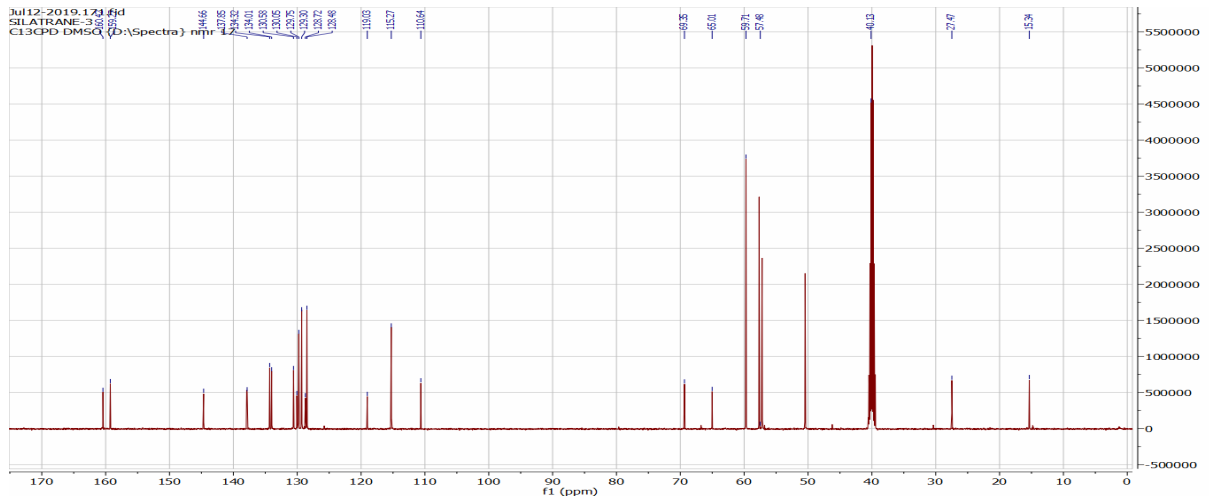
WATERS, Q-TOF MICROMASS (ESI-MS)

SANJAY ORTHOSILANE 22 (0.408) Cm (1:23)

SAIF/CIL, PANJAB UNIVERSITY, CHANDIGARH

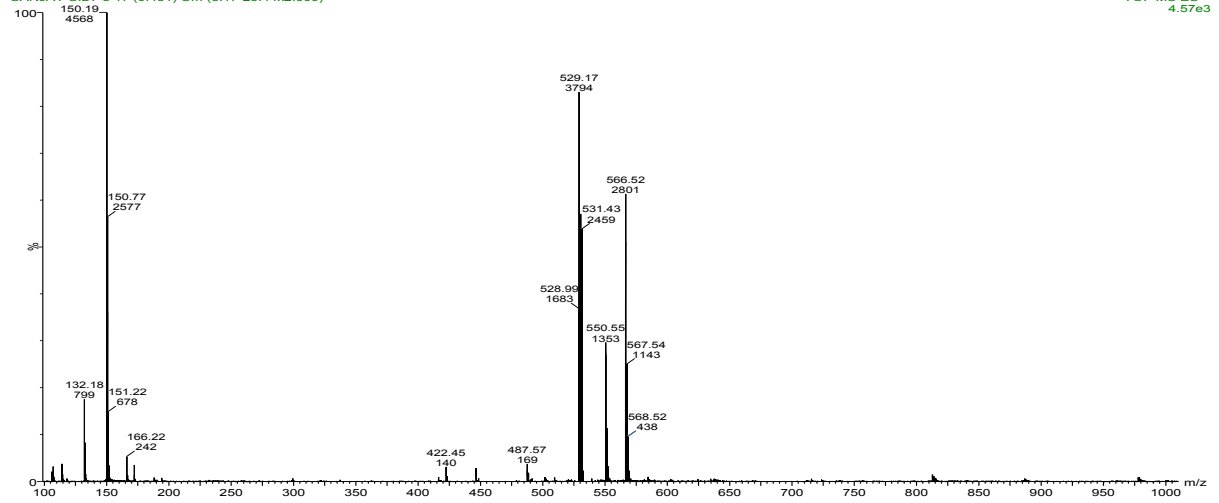
TOF MS ES+ 1.02e4



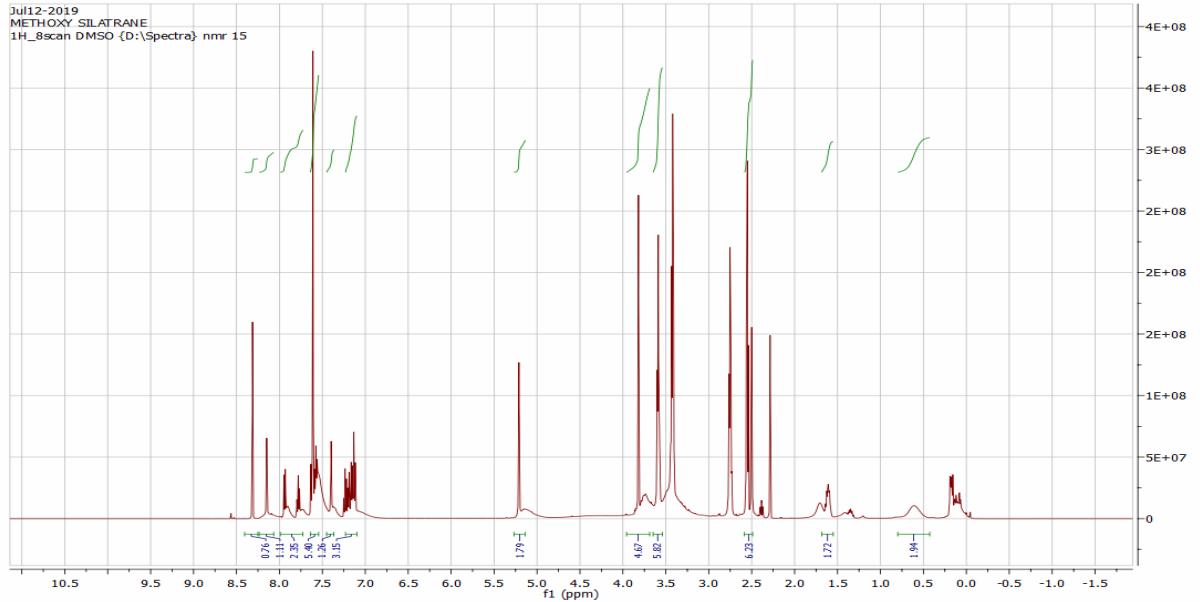


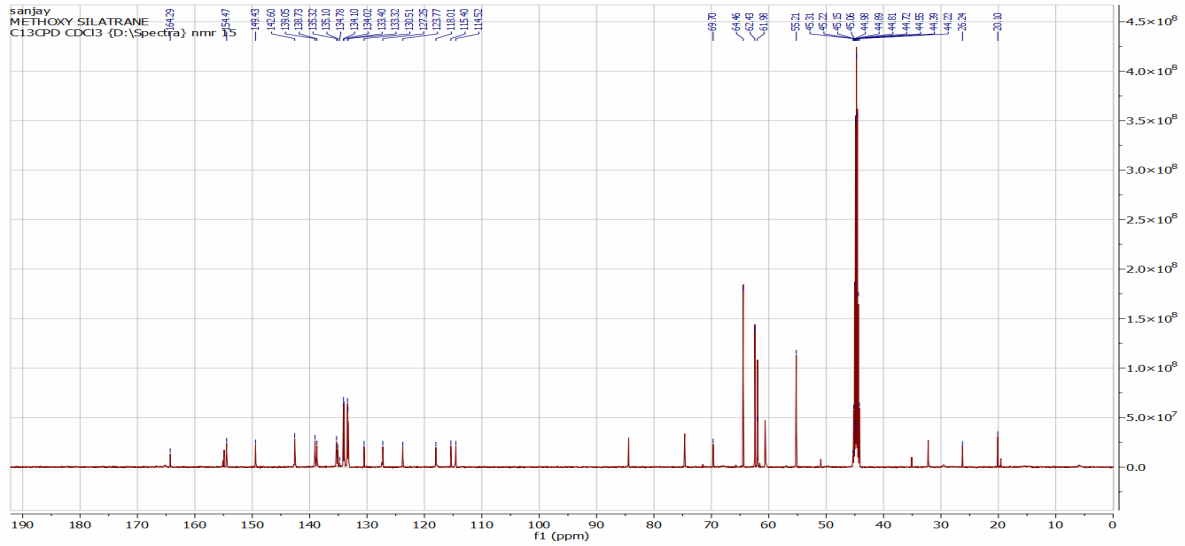
WATERS Q-TOF MICROMASS (ESI-MS)
 SANJAY SILT-3 17 (0.451) Cm (3:17-25:44x2.000)

SAIF/CIL, PANJAB UNIVERSITY, CHANDIGARH
 TOF MS ES+
 4.57e3



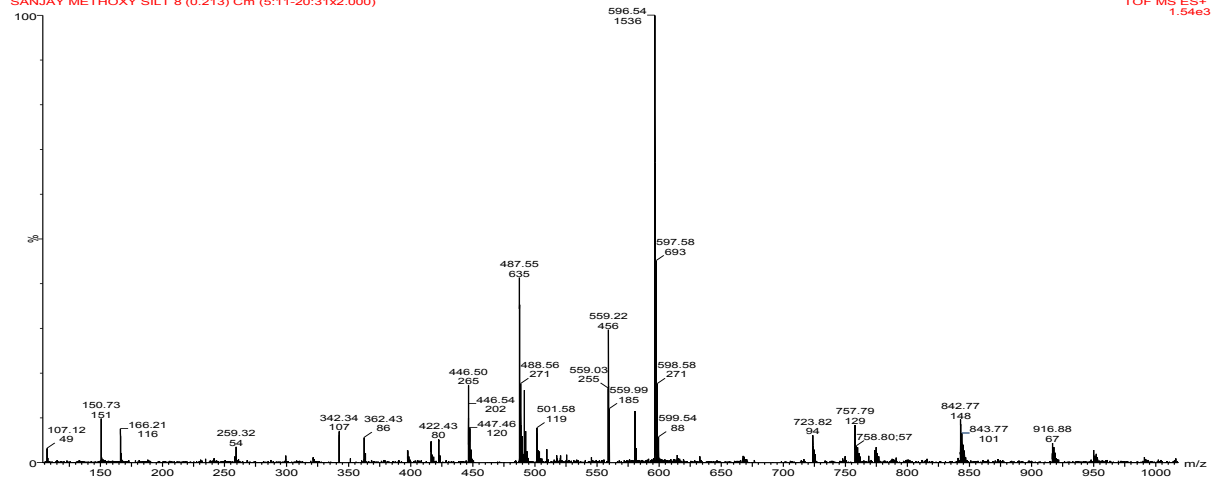
Jul12-2019
 METHOXY SILATRANE
 1H_8scan DMSO (D:\Spectra) nmr 15



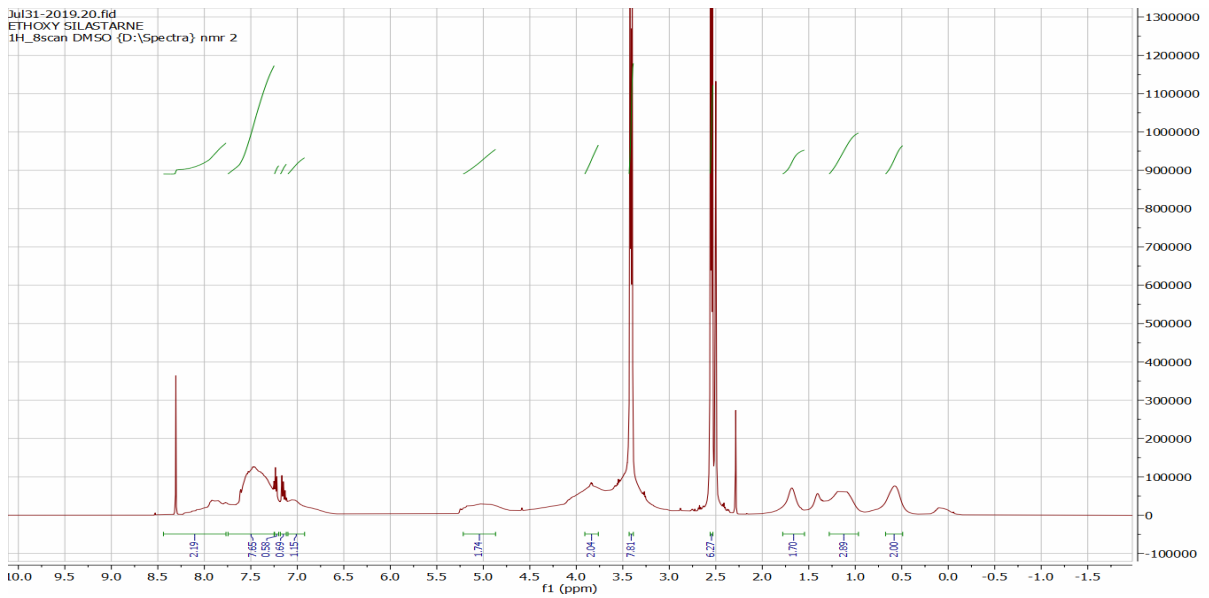


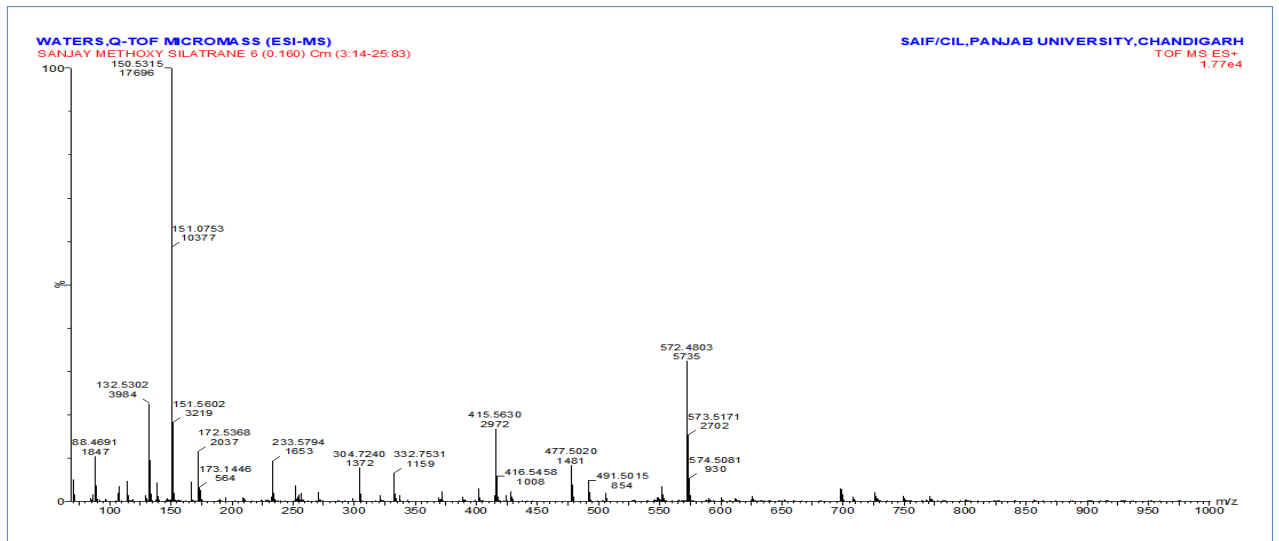
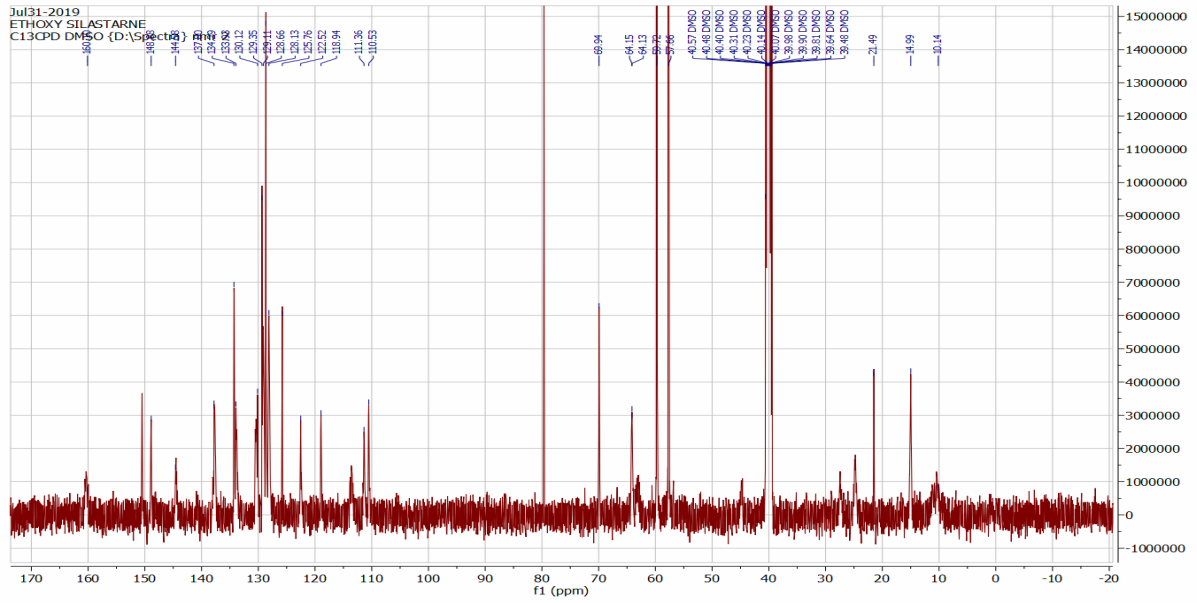
WATERS, Q-TOF MICROMASS (ESI-MS)
SANJAY METHOXY SILT 8 (0.213) Cm (5:11-20:31x2.000)

SAIF/CIL, PANJAB UNIVERSITY, CHANDIGARH
TOF MS ES+
1.54e3



Jul31-2019, 20.fid
ETHOXY SILASTARNE
1H_8scan DMSO (D:\Spectra) nmr 2





Selected bond lengths (Å) for 5 (c)

Parameter X-ray Parameter X-ray parameter

| | | | |
|--------|-------------|---------|------------|
| Si1 O3 | 1.6425 (18) | C16-C15 | 1.373 (3) |
| Si1 O1 | 1.647 (2) | C24C29 | 1.381 (4) |
| Si1 O2 | 1.656 (2) | C24C21 | 1.499 (3) |
| Si1 N1 | 2.182 (3) | C24C25 | 1.385 (4) |
| Si1 C7 | 1.866 (3) | C13C12 | 1.388 (3) |
| O4 C14 | 1.366 (3) | C29C28 | 1.396 (3) |
| O4 C17 | 1.405 (3) | C29C30 | 1.451 (4) |
| O3 C6 | 1.407 (3) | C28C27 | 1.365 (4) |
| N2 C10 | 1.251 (3) | C22C21 | 1.379 (3) |
| N2 C9 | 1.463 (3) | C2 C23 | 1.386 (3) |
| O1 C1 | 1.411 (4) | C27C26 | 1.370 (4) |
| O2 C4 | 1.404 (4) | C21C20 | 1.387 (4) |
| N1 C2A | 1.461 (6) | C18C23 | 1.382 (4) |
| N1 C2B | 1.530 (10) | C18C17 | 1.503 (3) |
| N1 C3A | 1.509 (6) | C18C19 | 1.368 (4) |
| N1 C3B | 1.391 (8) | C25C26 | 1.376 (3) |
| N1 C5A | 1.459 (10) | N3 C30 | 1.137 (4) |
| N1 C5B | 1.445 (9) | C20C19 | 1.379 (4) |
| C11C10 | 1.473 (3) | C4 C3A | 1.501 (6) |
| C11C16 | 1.389 (3) | C4 C3B | 1.635 (11) |
| C11C12 | 1.373 (3) | C6 C5A | 1.593 (11) |
| C14C13 | 1.377 (4) | C6 C5B | 1.400 (12) |
| C14C15 | 1.387 (4) | C1 C2A | 1.592 (7) |
| C8 C9 | 1.510 (4) | C1 C2B | 1.461 (8) |
| C8 C7 | 1.511 (4) | | |

Bond Angles for 5c

Atom AtomAtom Angle/ Atom Atom Atom Angle

| | | | | | |
|---------|---------|---------|-------------|---------------|-------------|
| O3 | Si1 | O1 | 119.35 (13) | C25 C24 C21 | 119.5 (3) |
| O3 | Si1 | O2 | 118.41 (12) | C14 C13 C12 | 119.5 (3) |
| O3 | Si1 | N1 | 81.88 (9) | C24 C29 C28 | 120.7 (3) |
| O3 | Si1 | C7 | 97.40 (11) | C24 C29 C30 | 122.7 (2) |
| O1 | Si1 | O2 | 117.03 (12) | C28 C29 C30 | 116.5 (3) |
| O1 | Si1 | N1 | 83.09 (10) | C11 C12 C13 | 121.9 (2) |
| O1 | Si1 | C7 | 98.29 (12) | N2 C9 C8 | 111.8 (2) |
| O2 | Si1 | N1 | 82.14 (11) | C16 C15 C14 | 120.5 (2) |
| O2 | Si1 | C7 | 97.19 (12) | C27 C28 C29 | 121.1 (3) |
| C7 | Si1 | N1 | 178.61 (11) | C8 C7 Si1 | 117.44 (19) |
| C14 | O4 | C17 | 117.3 (2) | C21 C22 C23 | 121.1 (2) |
| C6 | O3 | Si1 | 125.05 (19) | C28 C27 C26 | 118.4 (3) |
| C10 | N2 | C9 | 118.3 (2) | C22 C21 C24 | 123.7 (2) |
| C1 | O1 | Si1 | 123.7 (2) | C22 C21 C20 | 118.0 (2) |
| C4 | O2 | Si1 | 124.2 (2) | C20 C21 C24 | 118.2 (2) |
| C2 A | N1 | Si1 | 105.0 (3) | C23 C18 C17 | 124.3 (2) |
| C2 A | N1 | C3 A | 111.6 (4) | C19 C18 C23 | 118.2 (2) |
| C2B | N1 | Si1 | 101.1 (4) | C19 C18 C17 | 117.5 (2) |
| C3 A | N1 | Si1 | 104.1 (2) | C26 C25 C24 | 121.6 (3) |
| C3B | N1 | Si1 | 107.3 (4) | C27 C26 C25 | 121.0 (3) |
| C3B | N1 | C2B | 111.3 (6) | C18 C23 C22 | 120.5 (3) |
| C3B | N1 | C5B | 124.2 (7) | N3 C30 C29 | 177.1 (3) |
| C5 A | N1 | Si1 | 109.2 (5) | O4 C17 C18 | 111.1 (2) |
| C5 A | N1 | C2 A | 114.7 (5) | C19 C20 C21 | 120.4 (3) |
| C5 A | N1 | C3 A | 111.4 (5) | C18 C19 C20 | 121.8 (3) |
| C5B | N1 | Si1 | 103.3 (4) | O2 C4 C3 A | 110.6 (3) |
| C5B | N1 | C2B | 107.0 (6) | O2 C4 C3B | 109.5 (4) |
| C16 | C1 1 | C10 | 122.0 (2) | O3 C6 C5 A | 112.0 (4) |
| C12 | C1 1 | C10 | 120.1 (2) | C5 B C6 O3 | 111.8 (4) |
| C12 | C1 1 | C16 | 117.9 (2) | O1 C1 C2 A | 108.3 (3) |

| | | | | | | | |
|-----|---------|-----|----------|----|---------|-----|----------|
| N2 | C1 0 | C11 | 124.4(2) | O1 | C1 | C2B | 111.8(4) |
| O4 | C1 4 | C13 | 124.7(2) | N1 | C2 A | C1 | 103.0(4) |
| O4 | C1 4 | C15 | 116.1(2) | C1 | C2BN1 | | 106.1(5) |
| C13 | C1 4 | C15 | 119.3(2) | C4 | C3 A | N1 | 104.0(4) |
| C9 | C8 | C7 | 114.2(2) | N1 | C3B | C4 | 102.9(6) |
| C15 | C1 6 | C11 | 121.0(2) | N1 | C5 A | C6 | 101.7(6) |
| C29 | C2 4 | C21 | 123.3(2) | C6 | C5BN1 | | 112.7(7) |
| C29 | C2 4 | C25 | 117.2(2) | | | | |
