Electronic Supplementary Material (ESI) for New Journal of Chemistry.

First report of X-ray characterized Organosilatranes based receptor for electrochemical analysis of Al^{3+} ions

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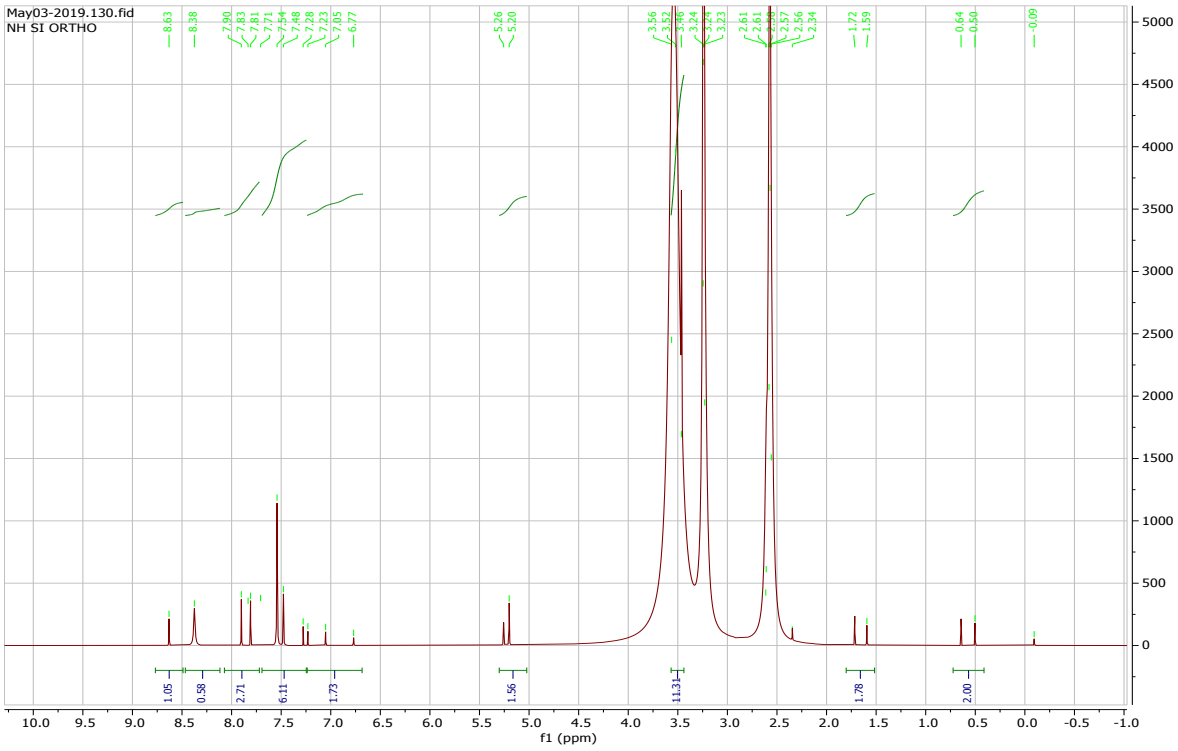
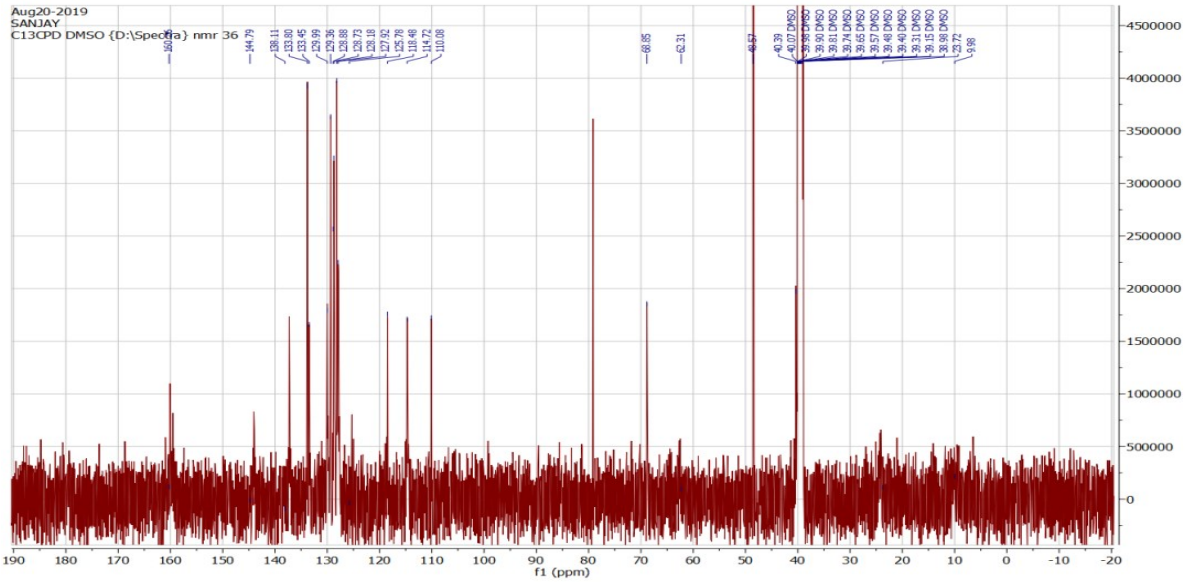
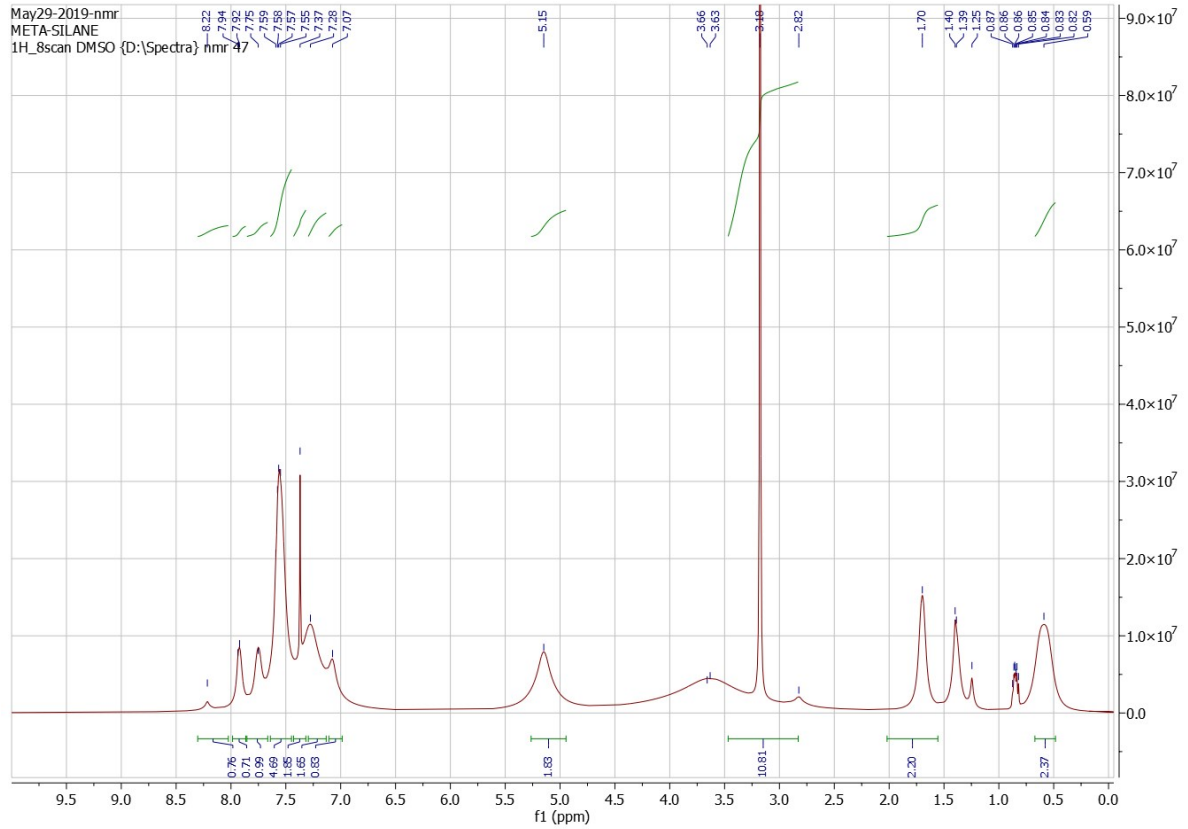



Aug20-2019
SANJAY
C13CPD DMSO {D:\Spectra} nmr 36
f1 (ppm)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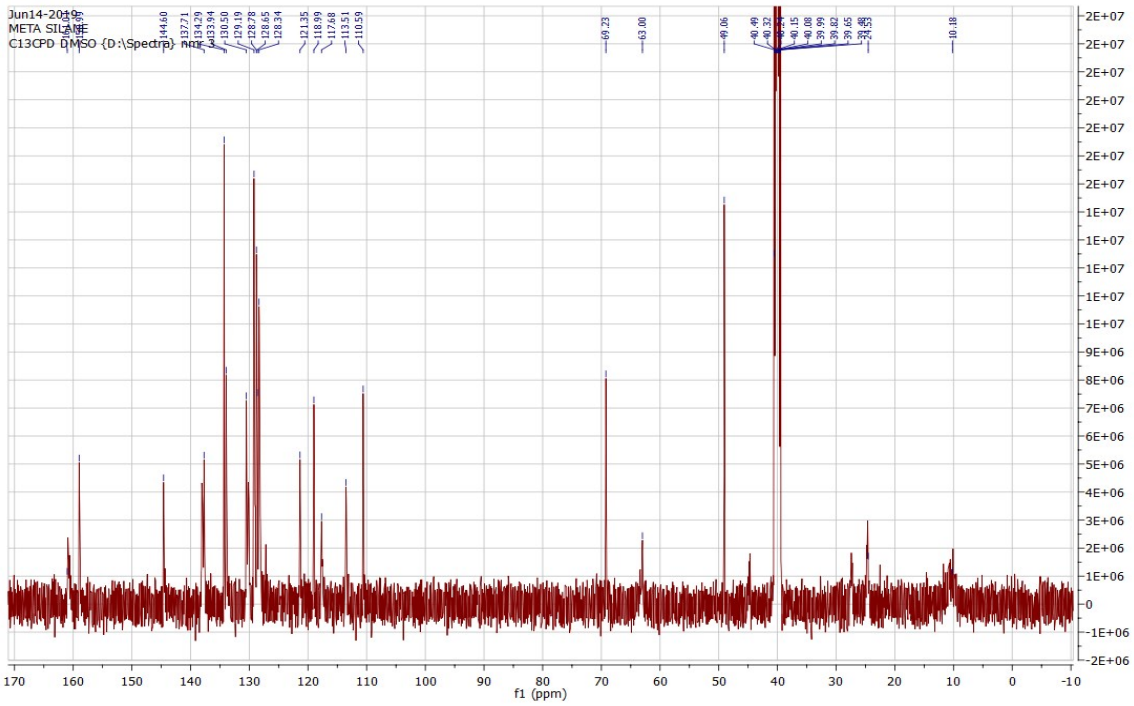
Jun14-2019
META SILANE
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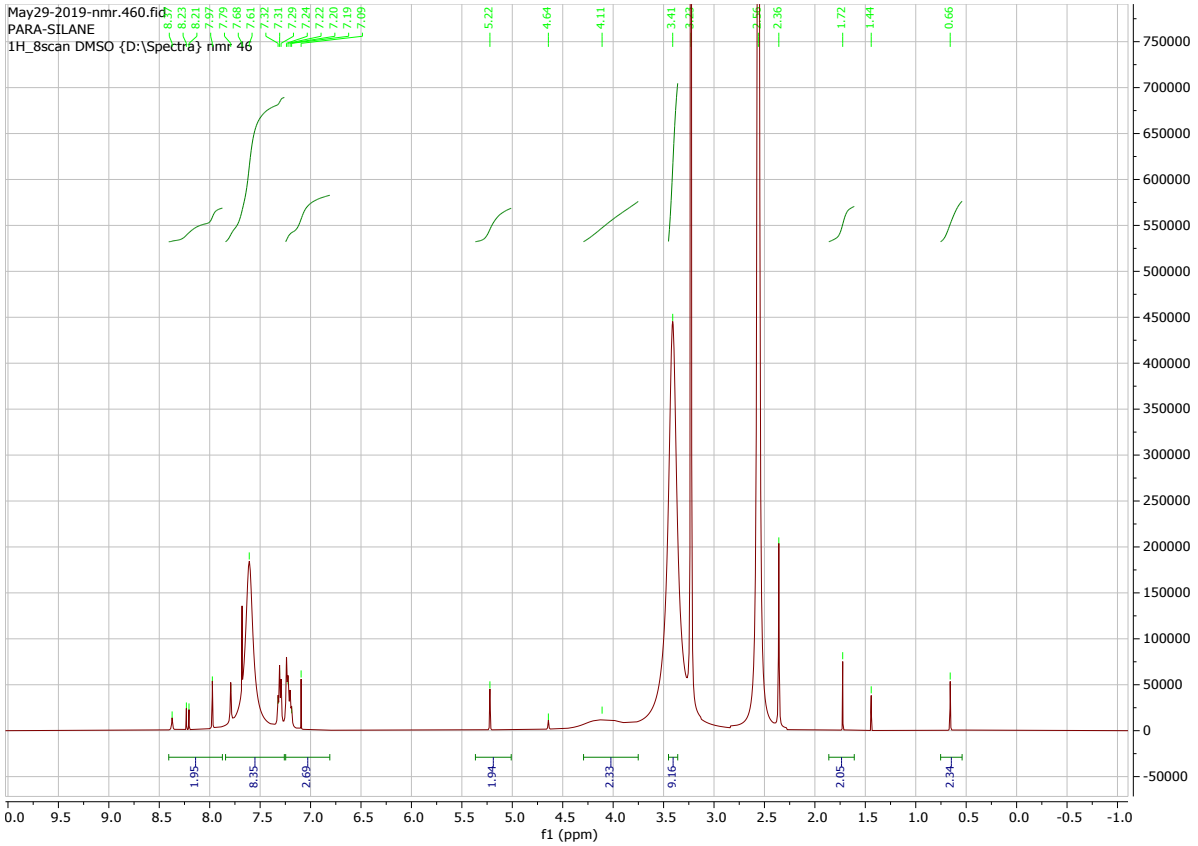
144.60
137.71
134.29
133.94
130.50
129.19
128.78
128.65
128.54
121.35
118.99
117.68
113.51
110.59
69.23
63.00
49.06
40.49
40.32
40.15
40.08
39.99
39.82
39.65
29.48
29.33
10.18
f1 (ppm)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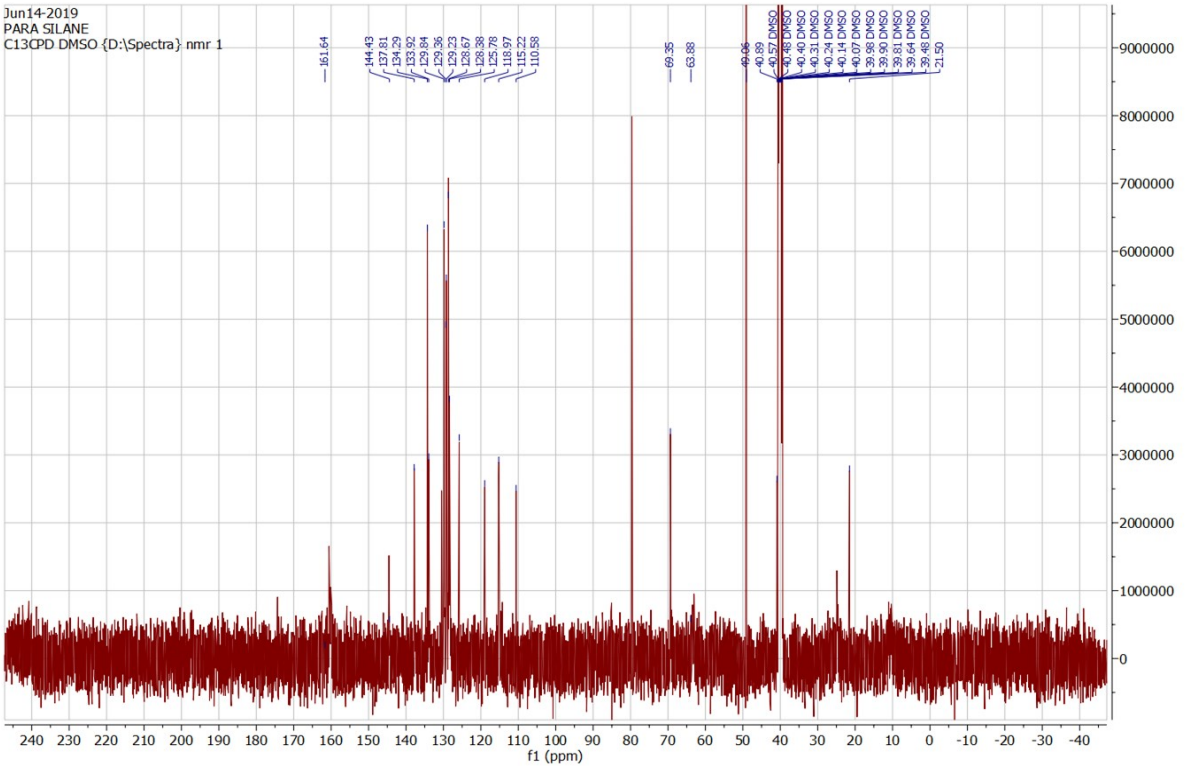
1H_8scan DMSO {D:\Spectra} nmr 46
f1 (ppm)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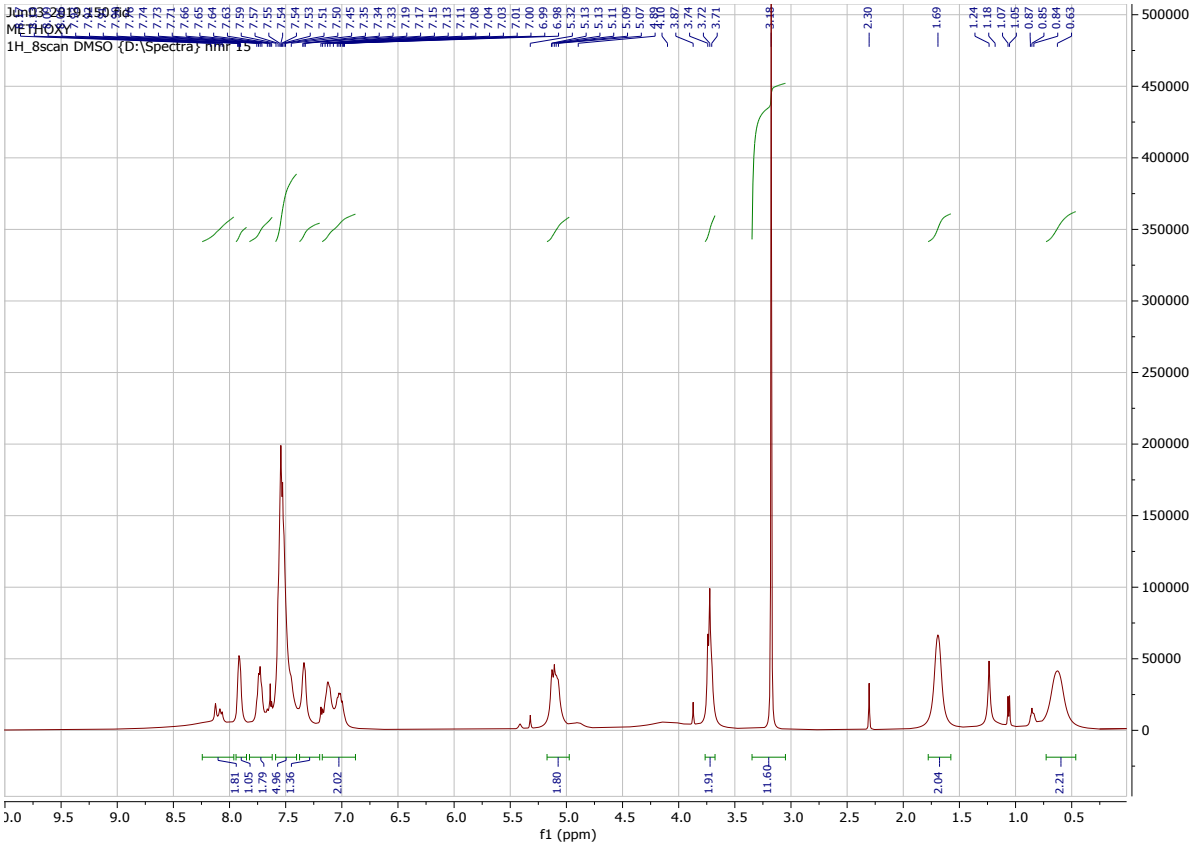
C13CPD DMSO {D:\Spectra} nmr 1
f1 (ppm)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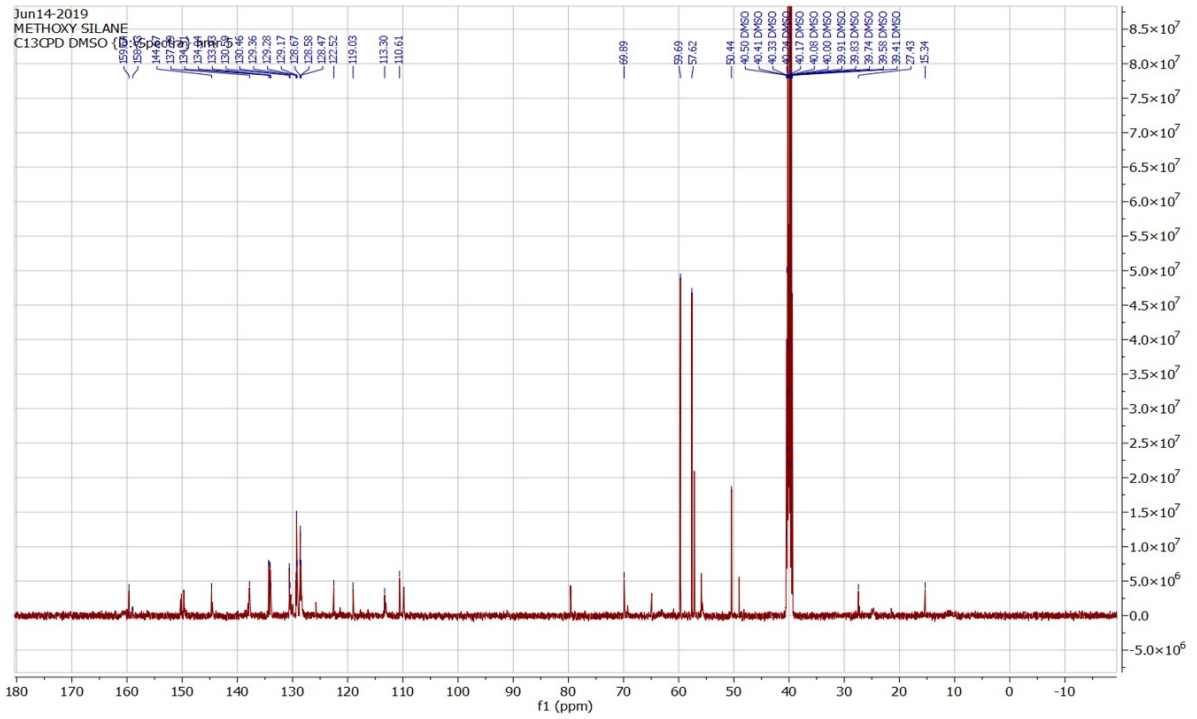
METHOXY
1H_8scan DMSO {D:\Spectra} nmr 15
f1 (ppm)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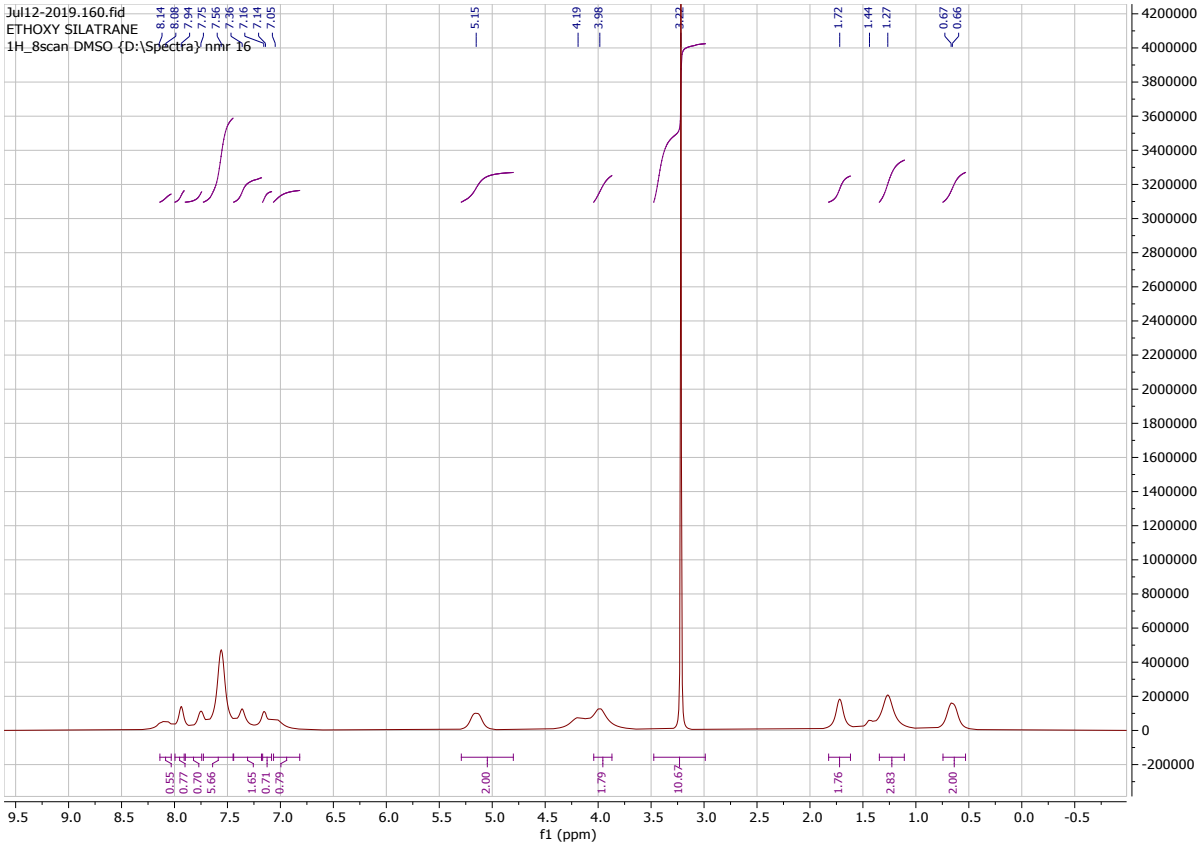
f1 (ppm)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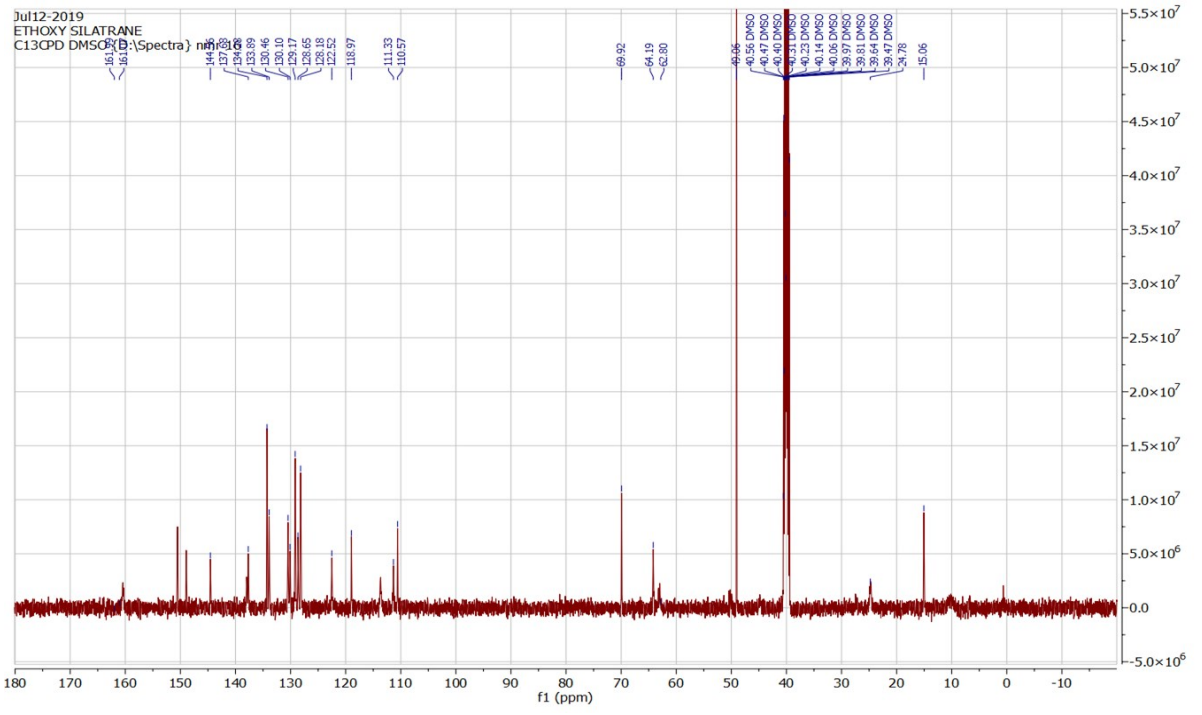
ETHOXY SILATRANE
1H_8scan DMSO {D:\Spectra} nmr 16
8.14
8.08
7.94
7.75
7.56
7.36
7.16
7.14
7.05
5.15
4.19
3.98
3.22
1.72
1.44
1.27
0.67
0.66
0.55
0.77
0.70
5.66
1.65
0.71
0.79
2.00
1.79
10.67
1.76
2.83
2.00
f1 (ppm)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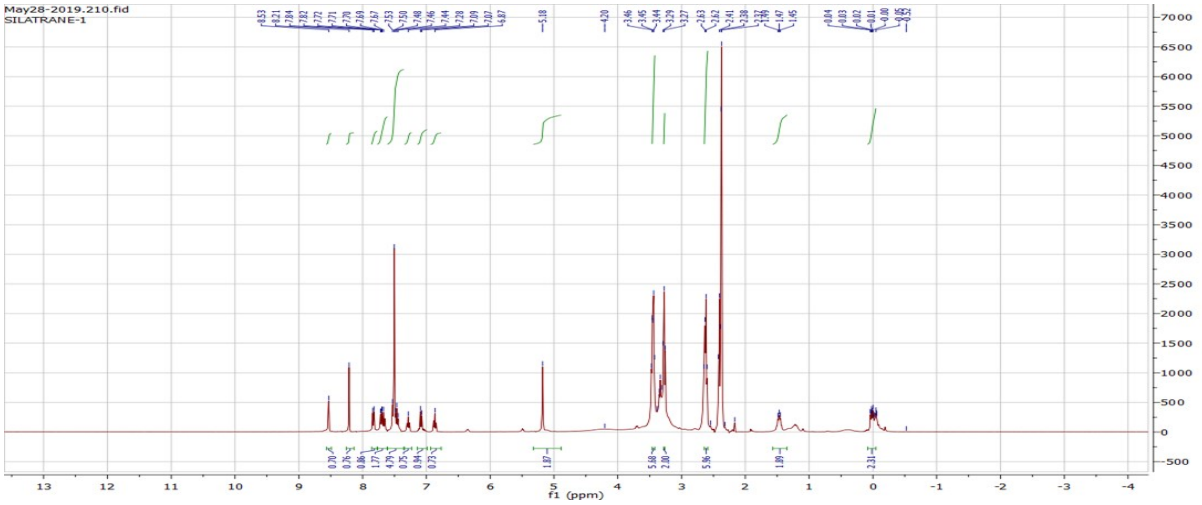
C13CPD DMSO {D:\Spectra} nmr 16
161.92
161.58
144.56
137.68
134.08
133.89
130.46
130.10
129.17
128.65
128.18
122.52
118.97
111.33
110.57
69.92
64.19
62.80
40.06
40.56 DMSO
40.40 DMSO
40.23 DMSO
40.14 DMSO
40.06 DMSO
39.97 DMSO
39.81 DMSO
39.64 DMSO
39.47 DMSO
24.78
15.06
f1 (ppm)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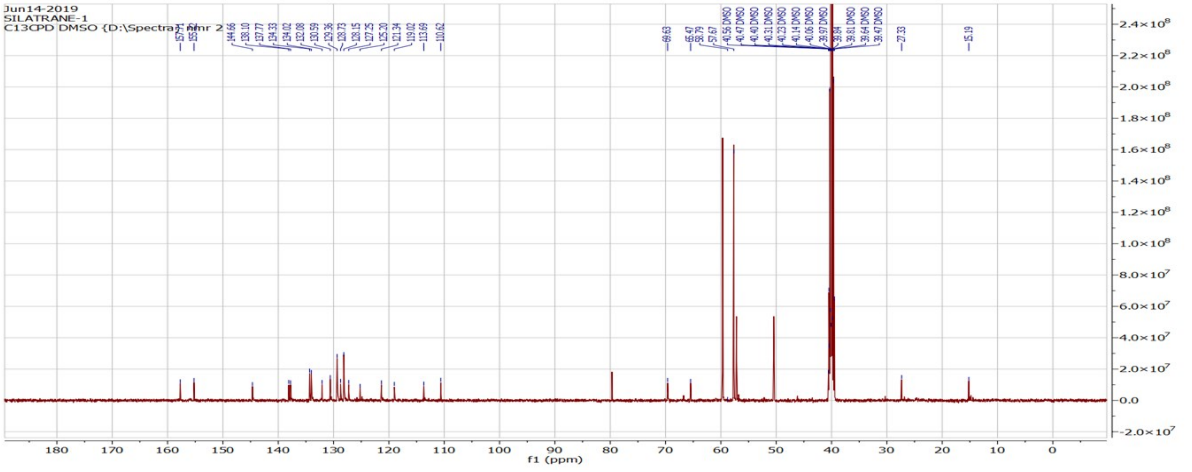
f1 (ppm)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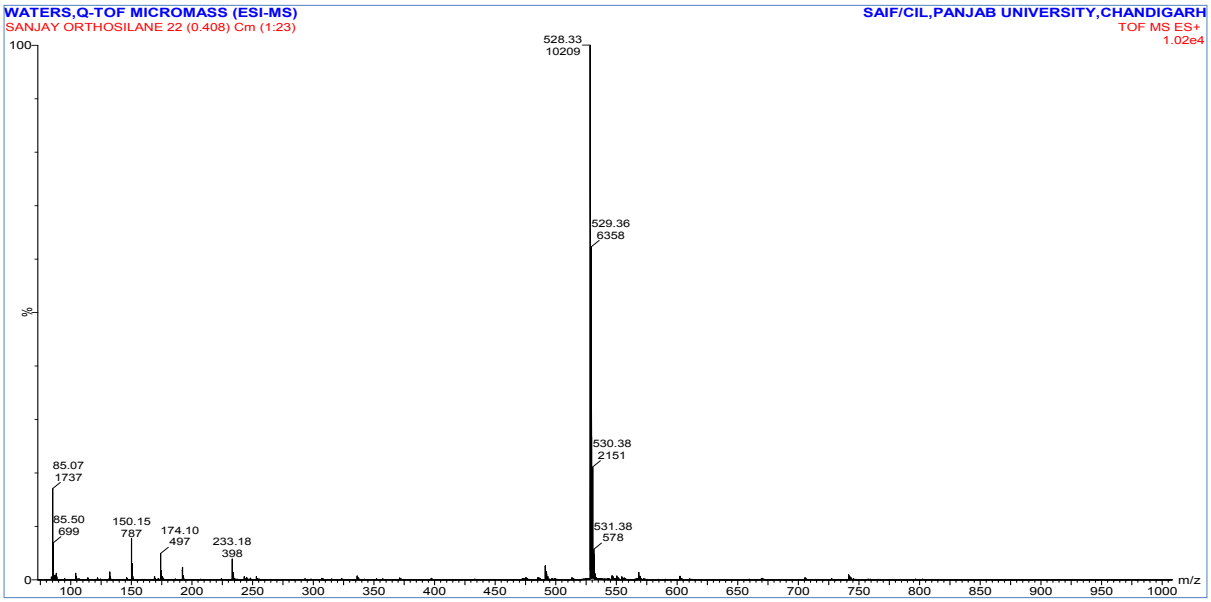
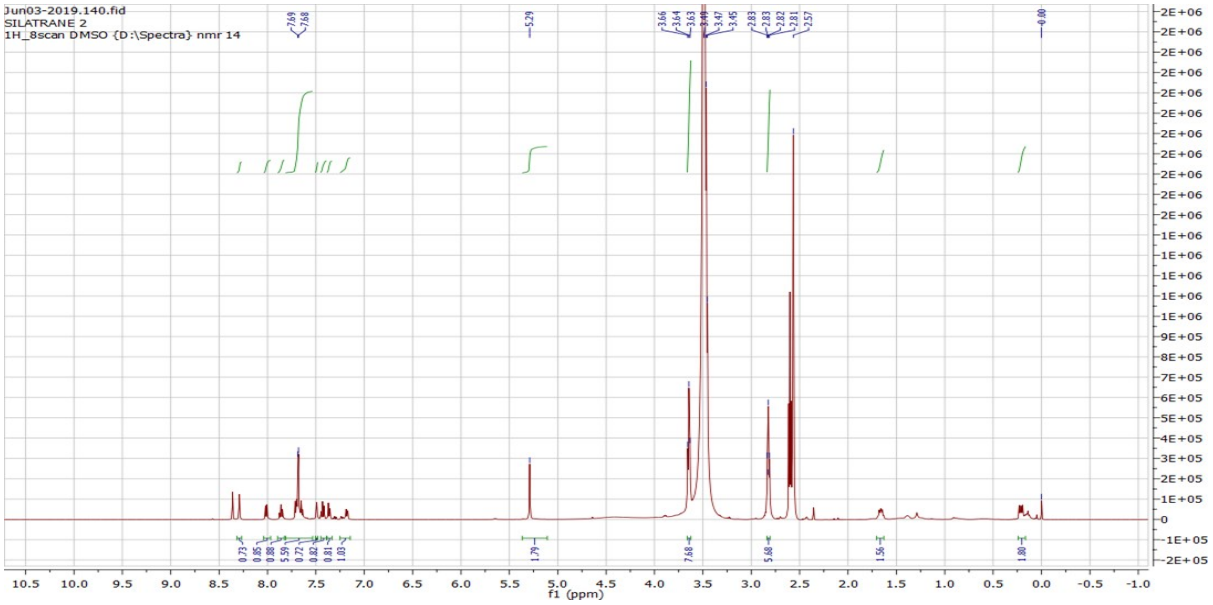
C13CPD DMSO {D:\Spectra} 5mm 2
f1 (ppm)


WATERS,Q-TOF MICROMASS (ESI-MS)
SANJAY ORTHOSILANE 22 (0.408) Cm (1:23)
SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH
TOF MS ES+
1.02e4
528.33
10209
529.36
6358
530.38
2151
531.38
578
85.07
1737
85.50
699
150.15
787
174.10
497
233.18
398
%
m/z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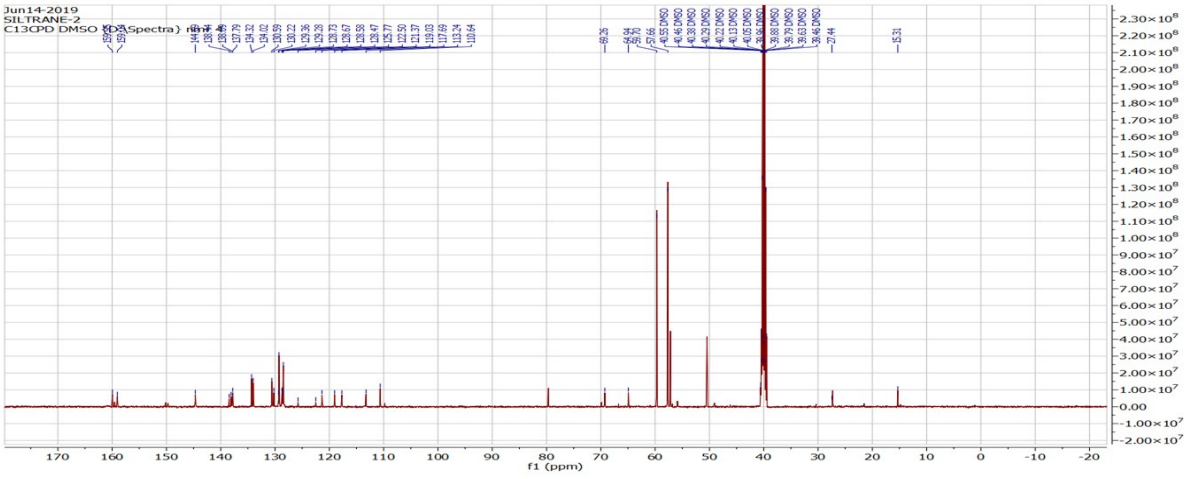
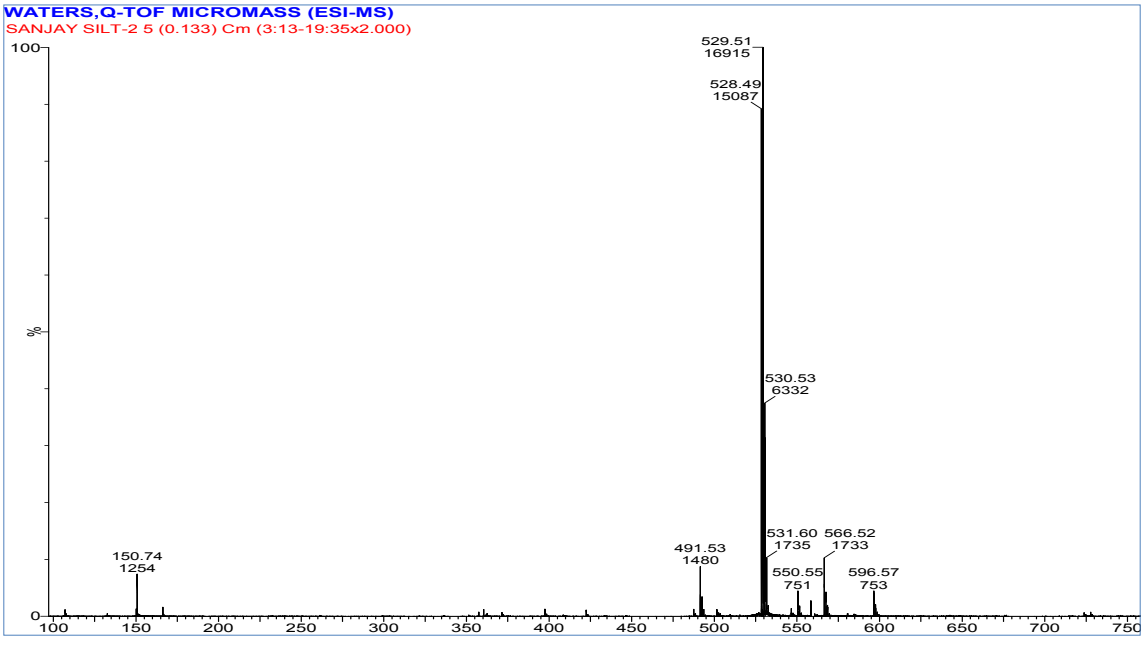
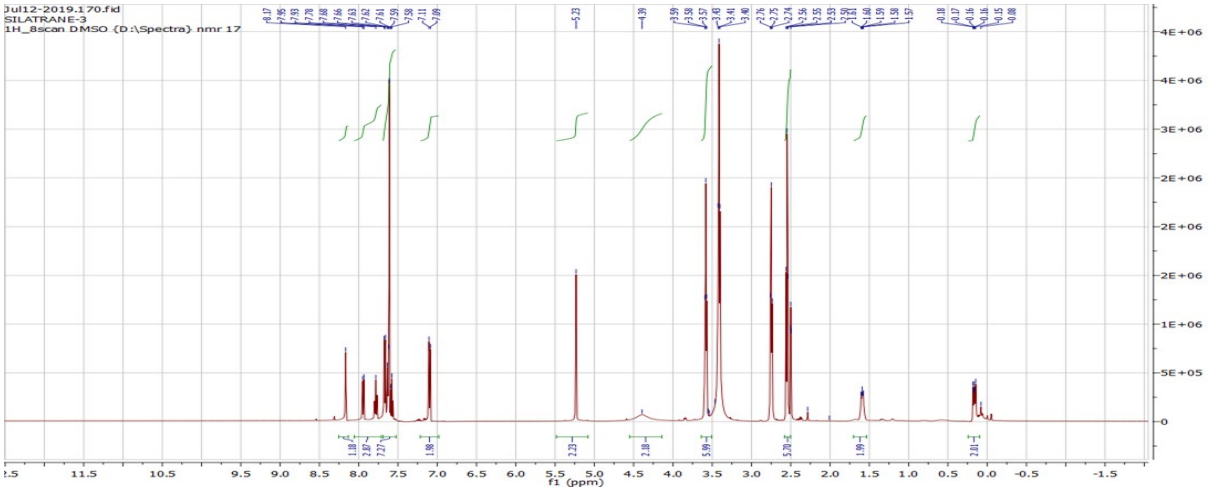
SILATRANE 2
1H_8scan DMSO {D:\Spectra} nmr 14
f1 (ppm)


Jun14-2019
SILATRANE-2
f1 (ppm)


WATERS,Q-TOF MICROMASS (ESI-MS)
SANJAY SILT-2 5 (0.133) Cm (3:13-19:35x2.000)
529.51
16915
528.49
15087
530.53
6332
531.60
1735
566.52
1733
491.53
1480
550.55
751
596.57
753
150.74
1254
%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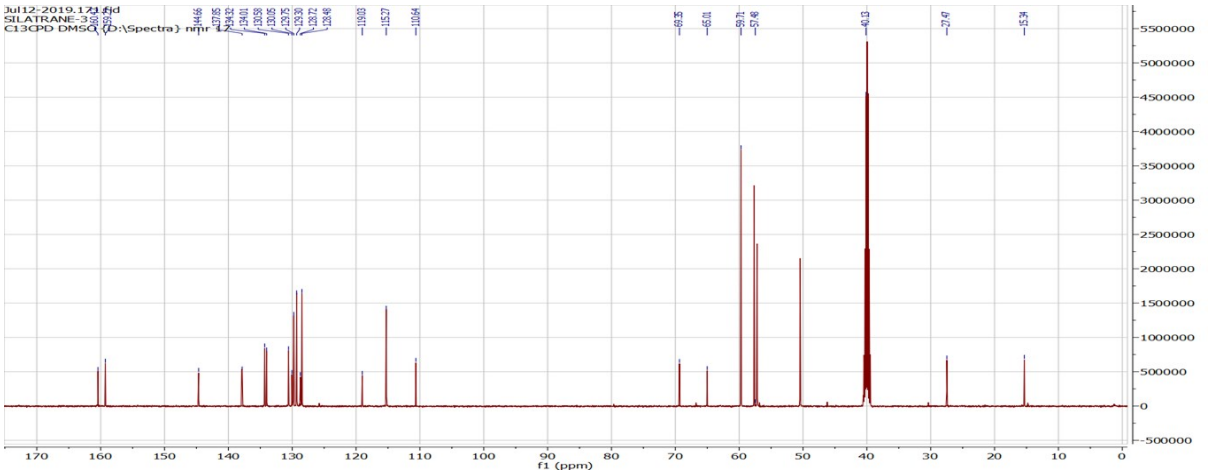
SILATRANE-3
1H_8scan DMSO (D:\Spectra) nmr 17
f1 (ppm)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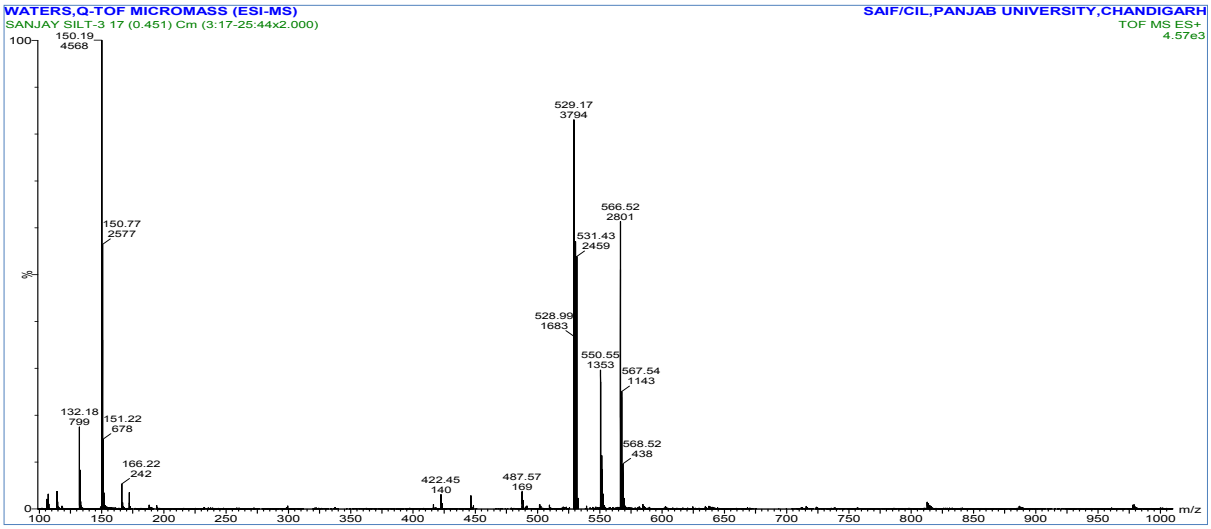
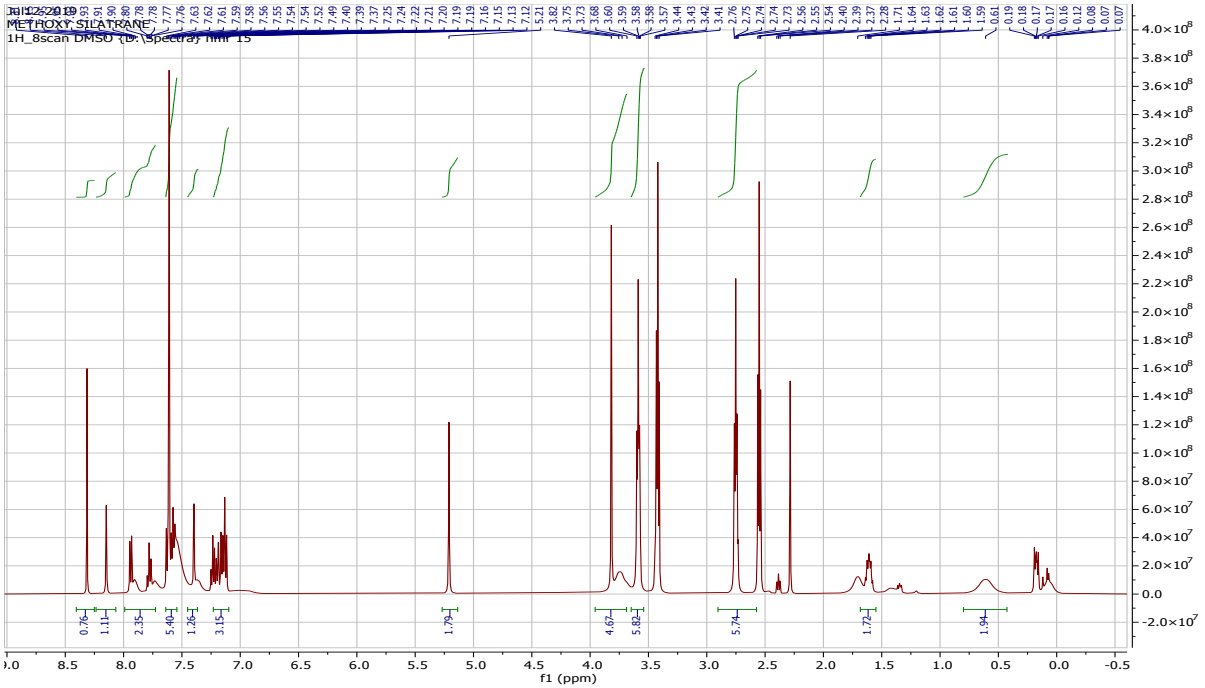
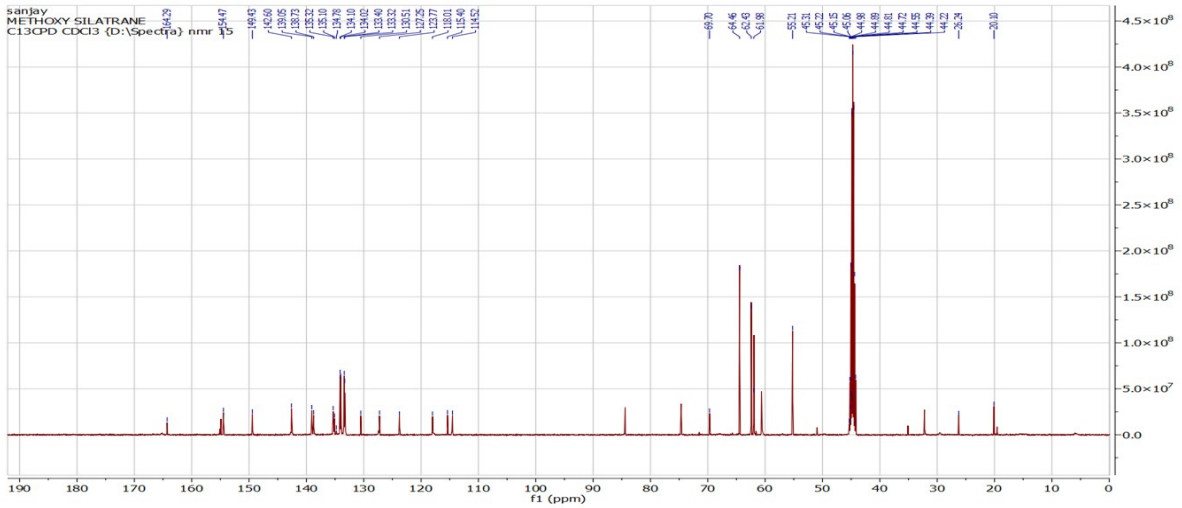
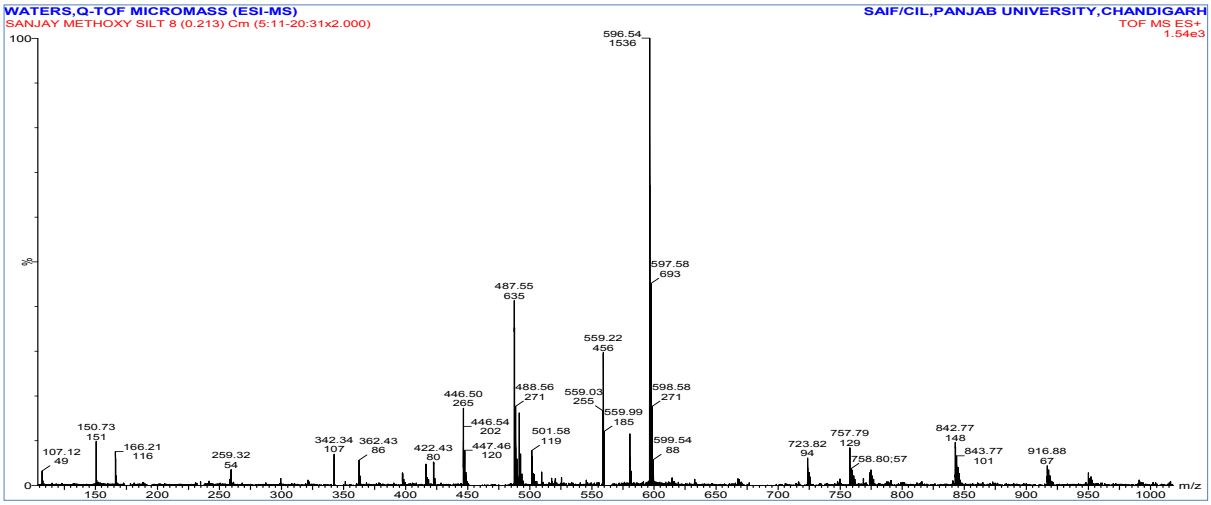
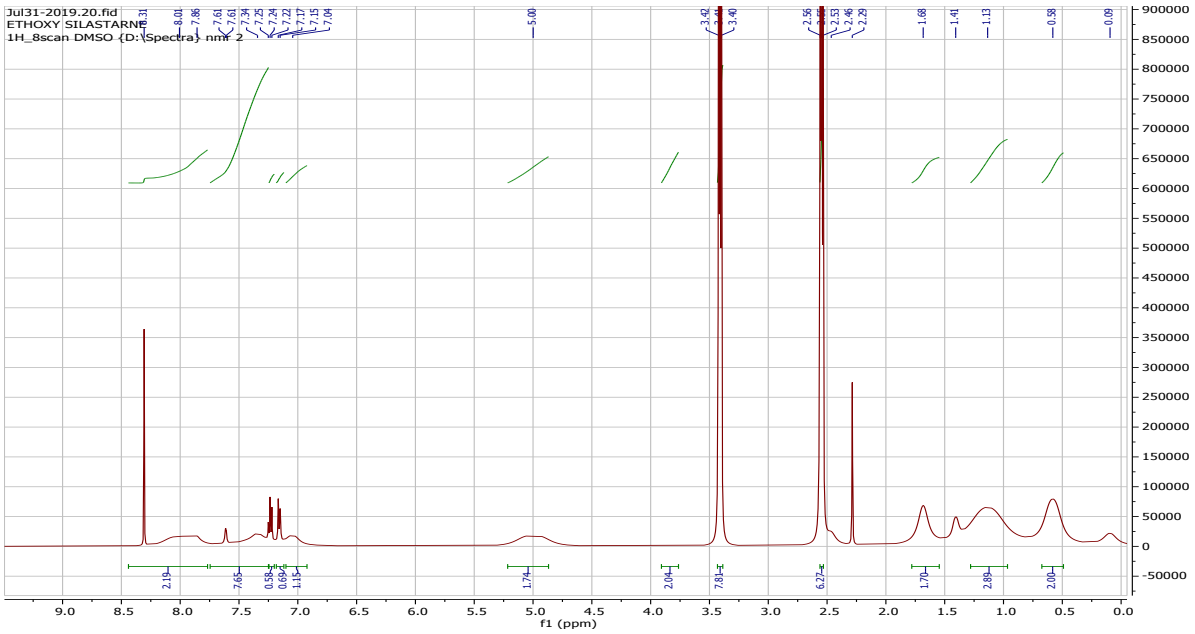
SILATRANE-3
C13CPD DMSO (D:\Spectra) nmr 17
f1 (ppm)


WATERS,Q-TOF MICROMASS (ESI-MS)
SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH
SANJAY SILT-3 17 (0.451) Cm (3:17-25:44x2.000)
TOF MS ES+
4.57e3
150.19
4568
529.17
3794
566.52
2801
150.77
2577
531.43
2459
528.99
1683
550.55
1353
567.54
1143
132.18
799
151.22
678
568.52
438
166.22
242
422.45
140
487.57
169
%
m/z


METHOXY SILATRANE
1H_8scan DMSO {D:\Spectra} nmr 15
f1 (ppm)


sanjay
METHOXY SILATRANE
C13CPD CDCl3 {D:\Spectra} nmr 15
f1 (ppm)


WATERS,Q-TOF MICROMASS (ESI-MS)
SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH
SANJAY METHOXY SILT 8 (0.213) Cm (5:11-20:31x2.000)
TOF MS ES+
1.54e3
596.54
1536
597.58
693
487.55
635
559.22
456
488.56
271
559.03
255
598.58
271
446.50
265
559.99
185
446.54
202
501.58
119
599.54
88
447.46
120
342.34
107
362.43
86
422.43
80
150.73
151
107.12
49
166.21
116
259.32
54
723.82
94
757.79
129
758.80;57
842.77
148
843.77
101
916.88
67
%
m/z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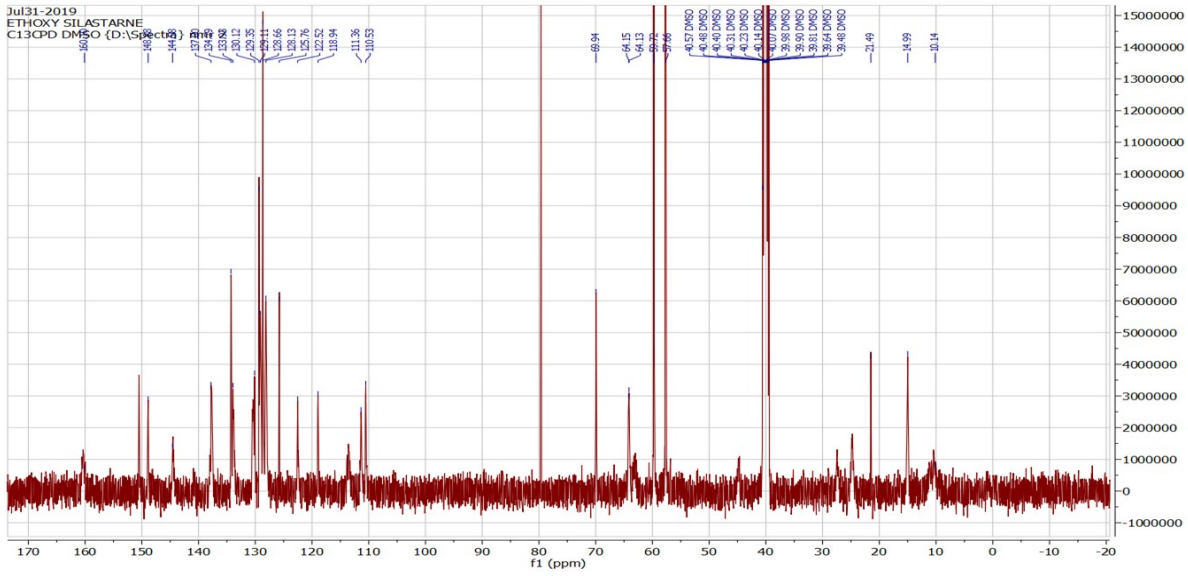
ETHOXY SILASTARNE
1H_8scan DMSO {D:\Spectra} nmr 2
f1 (ppm)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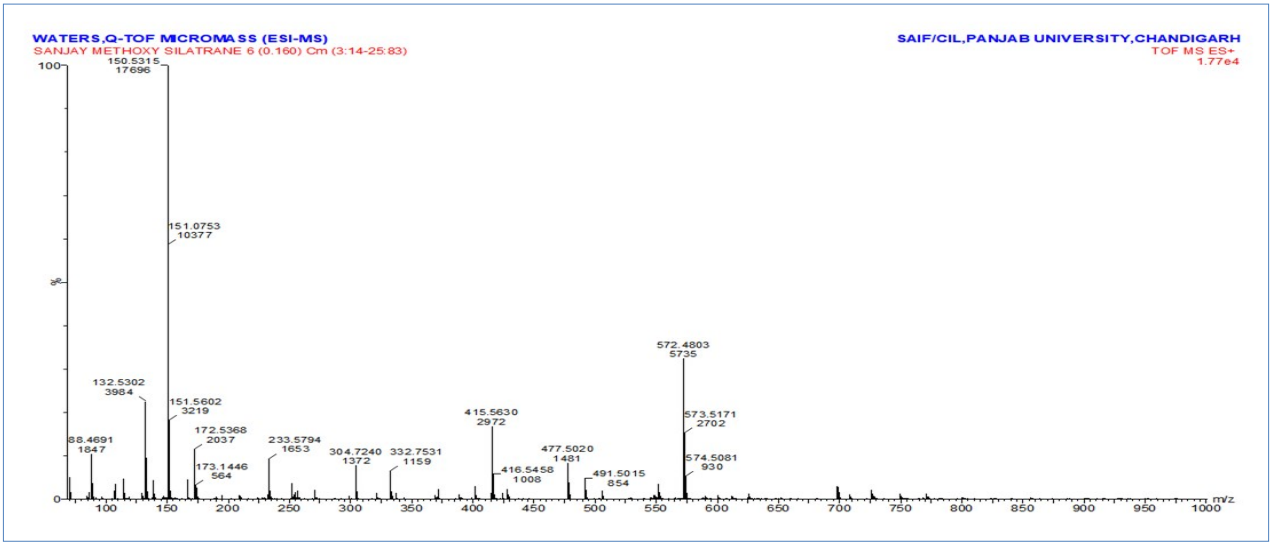
ETHOXY SILASTARNE
C13CPD DMSO {D:\Spectra} nmr
f1 (ppm)


WATERS,Q-TOF MICROMASS (ESI-MS)
SANJAY METHOXY SILATRANE 6 (0.160) Cm (3:14-25:83)
SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH
TOF MS ES+
1.77e4
150.5315
17696
151.0753
10377
132.5302
3984
151.5602
3219
172.5368
2037
88.4691
1847
173.1446
564
233.5794
1653
304.7240
1372
332.7531
1159
415.5630
2972
416.5458
1008
477.5020
1481
491.5015
854
572.4803
5735
573.5171
2702
574.5081
930
m/z

Selected bond lengths (Å) for 5 (c)

Parameter	X-ray	Parameter	Parameter	X-ray	parameter
Si1 O3	1.6425(18)	C16	-C15	1.373(3)	
Si1 O1	1.647(2)	C24	C29	1.381(4)	
Si1 O2	1.656(2)	C24	C21	1.499(3)	
Si1 N1	2.182(3)	C24	C25	1.385(4)	
Si1 C7	1.866(3)	C13	C12	1.388(3)	
O4 C14	1.366(3)	C29	C28	1.396(3)	
O4 C17	1.405(3)	C29	C30	1.451(4)	
O3 C6	1.407(3)	C28	C27	1.365(4)	
N2 C10	1.251(3)	C22	C21	1.379(3)	
N2 C9	1.463(3)	C2	C23	1.386(3)	
O1 C1	1.411(4)	C27	C26	1.370(4)	
O2 C4	1.404(4)	C21	C20	1.387(4)	
N1 C2A	1.461(6)	C18	C23	1.382(4)	
N1 C2B	1.530(10)	C18	C17	1.503(3)	
N1 C3A	1.509(6)	C18	C19	1.368(4)	
N1 C3B	1.391(8)	C25	C26	1.376(3)	
N1 C5A	1.459(10)	N3	C30	1.137(4)	
N1 C5B	1.445(9)	C20	C19	1.379(4)	
C11	C10	1.473(3)	C4	C3A	1.501(6)
C11	C16	1.389(3)	C4	C3B	1.635(11)
C11	C12	1.373(3)	C6	C5A	1.593(11)
C14	C13	1.377(4)	C6	C5B	1.400(12)
C14	C15	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

C5B	N1	Si1	103.3(4)	O2	C4	C3A	110.6(3)
C5B	N1	C2B	107.0(6)	O2	C4	C3B	109.5(4)
C16	C11	C10	122.0(2)	O3	C6	C5A	112.0(4)
C12	C11	C10	120.1(2)	C5B	C6	O3	111.8(4)
C12	C11	C16	117.9(2)	O1	C1	C2A	108.3(3)
N2	C10	C11	124.4(2)	O1	C1	C2B	111.8(4)
O4	C14	C13	124.7(2)	N1	C2A	C1	103.0(4)
O4	C14	C15	116.1(2)	C1	C2B	N1	106.1(5)
C13	C14	C15	119.3(2)	C4	C3A	N1	104.0(4)
C9	C8	C7	114.2(2)	N1	C3B	C4	102.9(6)
C15	C16	C11	121.0(2)	N1	C5A	C6	101.7(6)
C29	C24	C21	123.3(2)	C6	C5B	N1	112.7(7)
C29	C24	C25	117.2(2)				