Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Design and Synthesis of Novel Fluorescent Organosilicon-Based Chemosensors Through Click Silylation: Detection of Biogenic Amines

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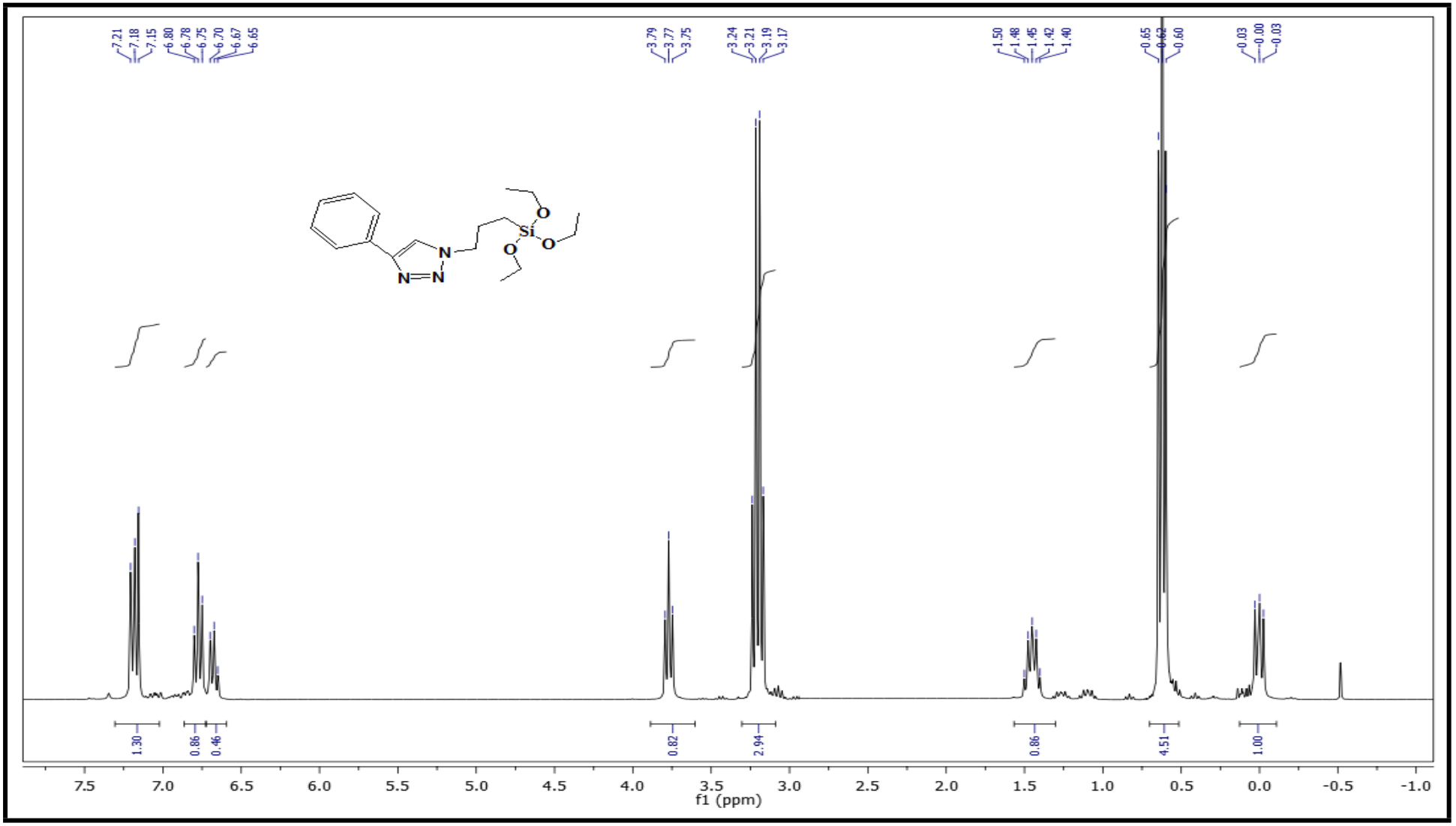
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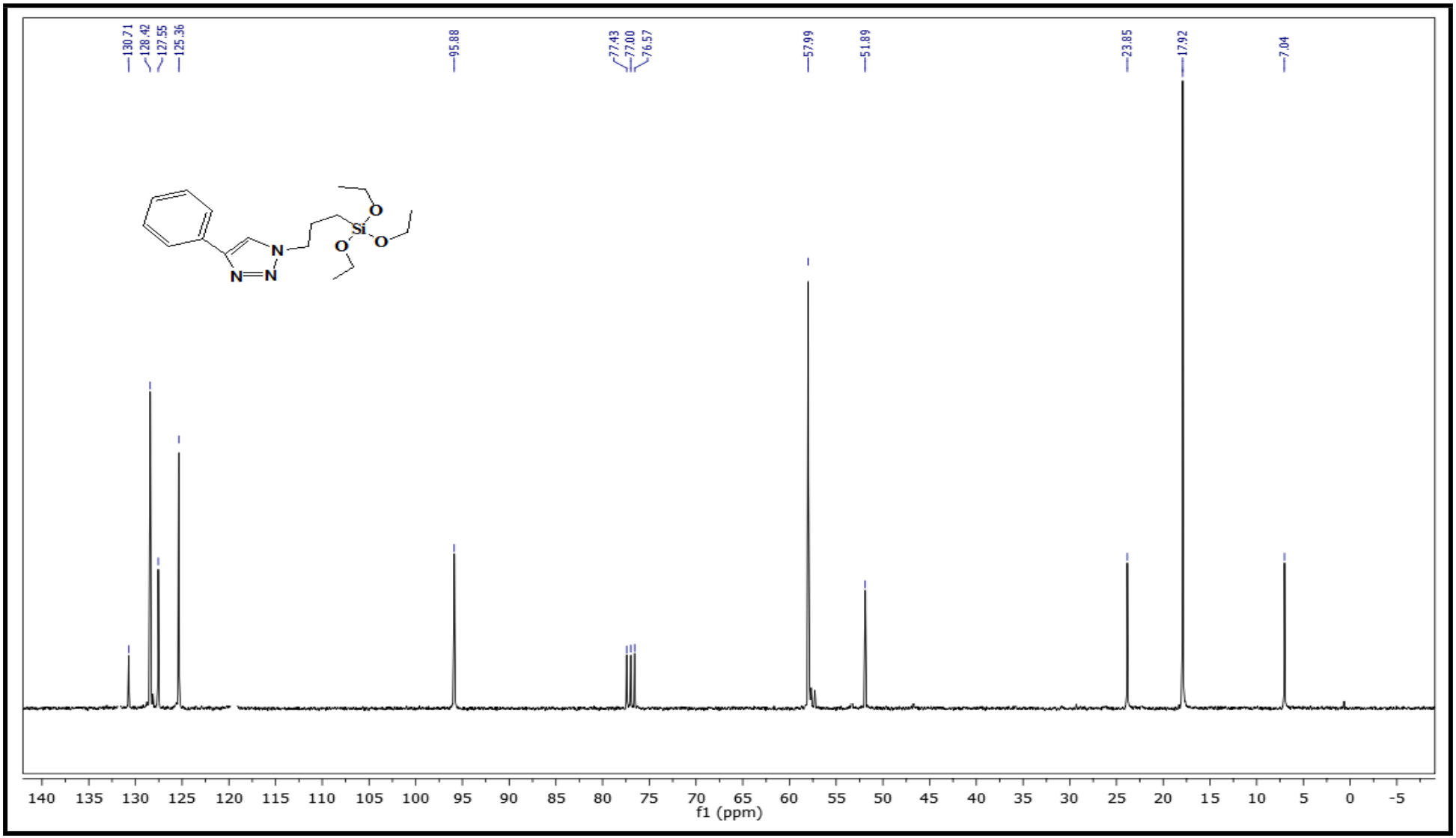
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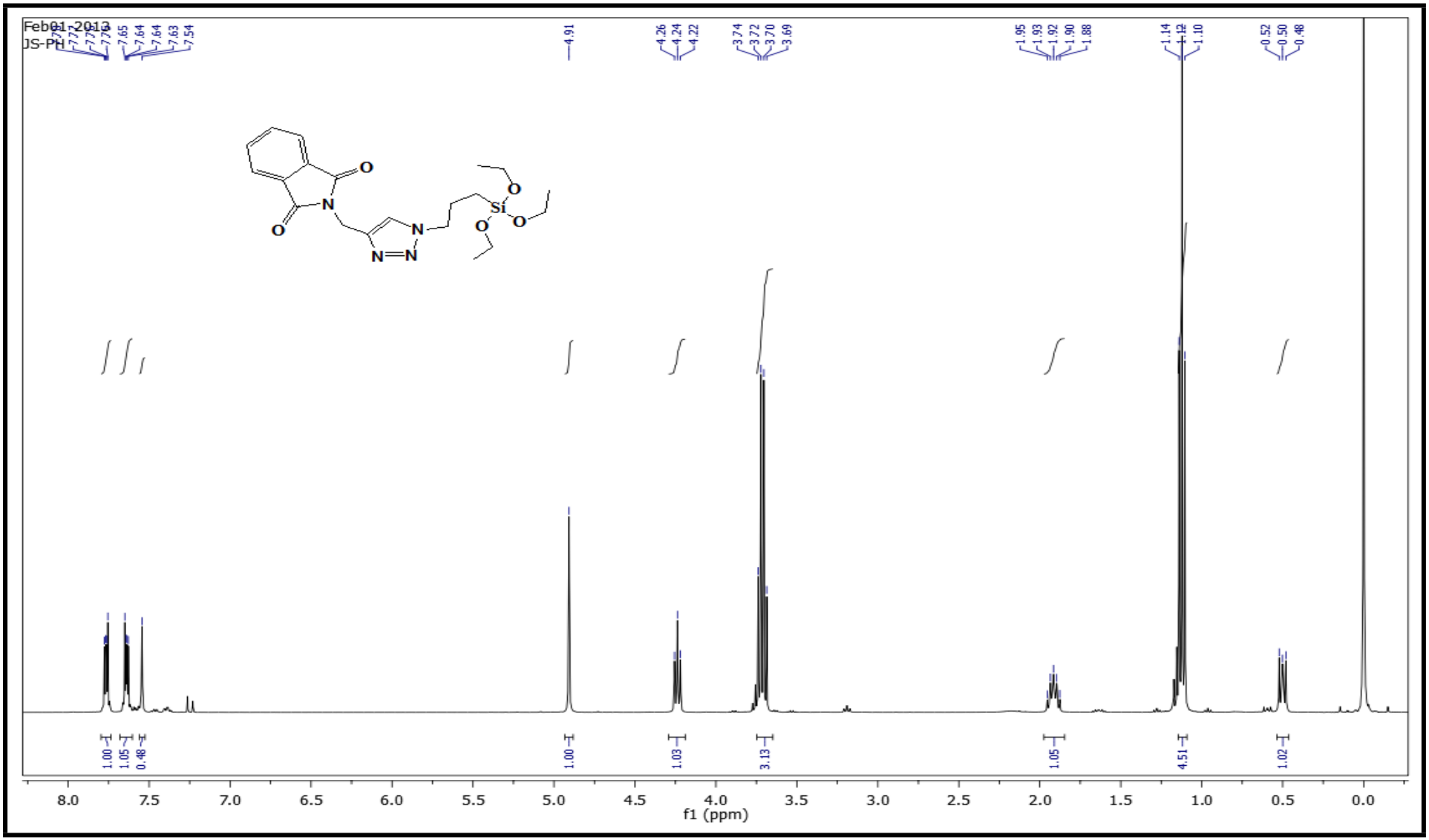
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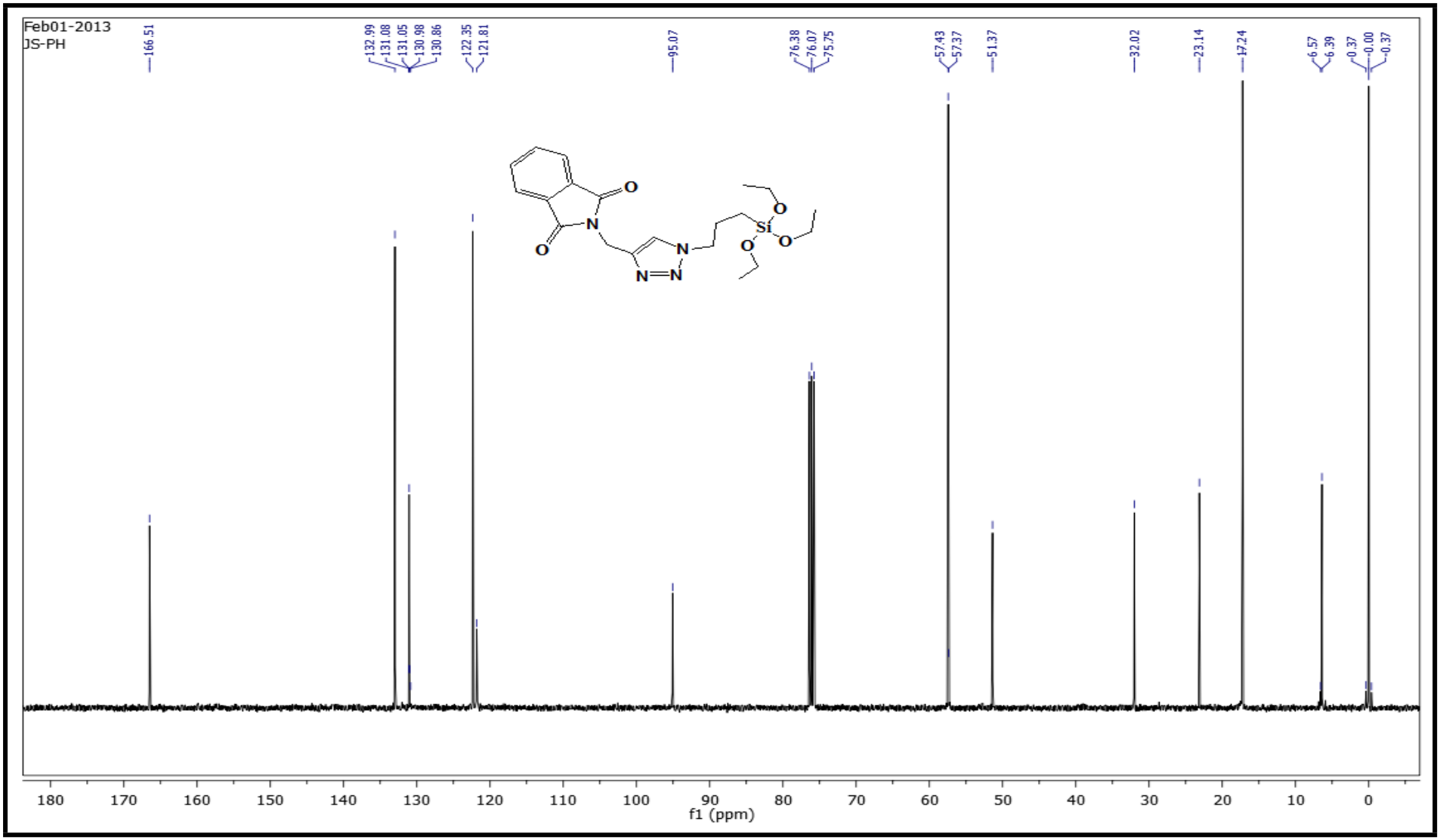
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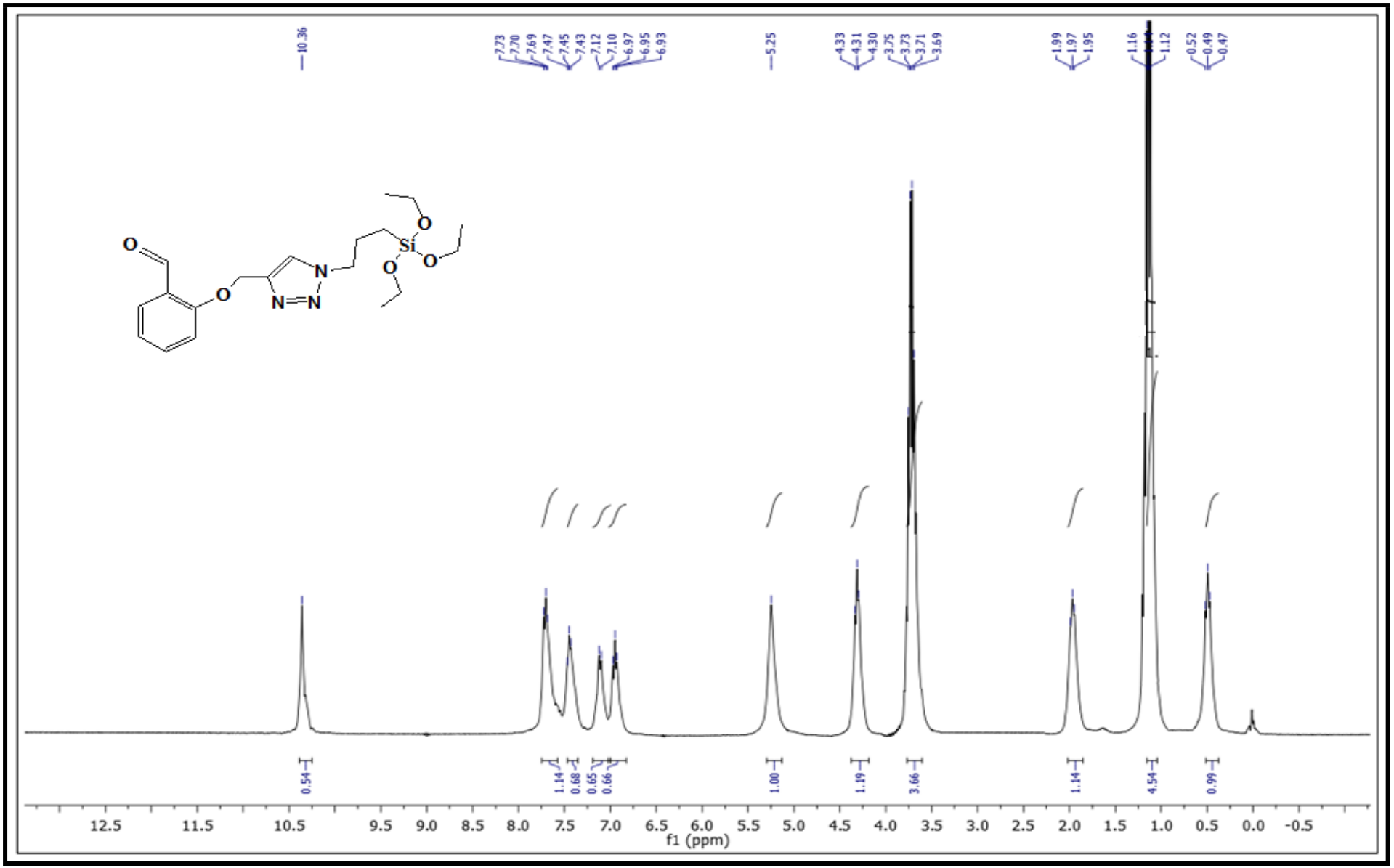
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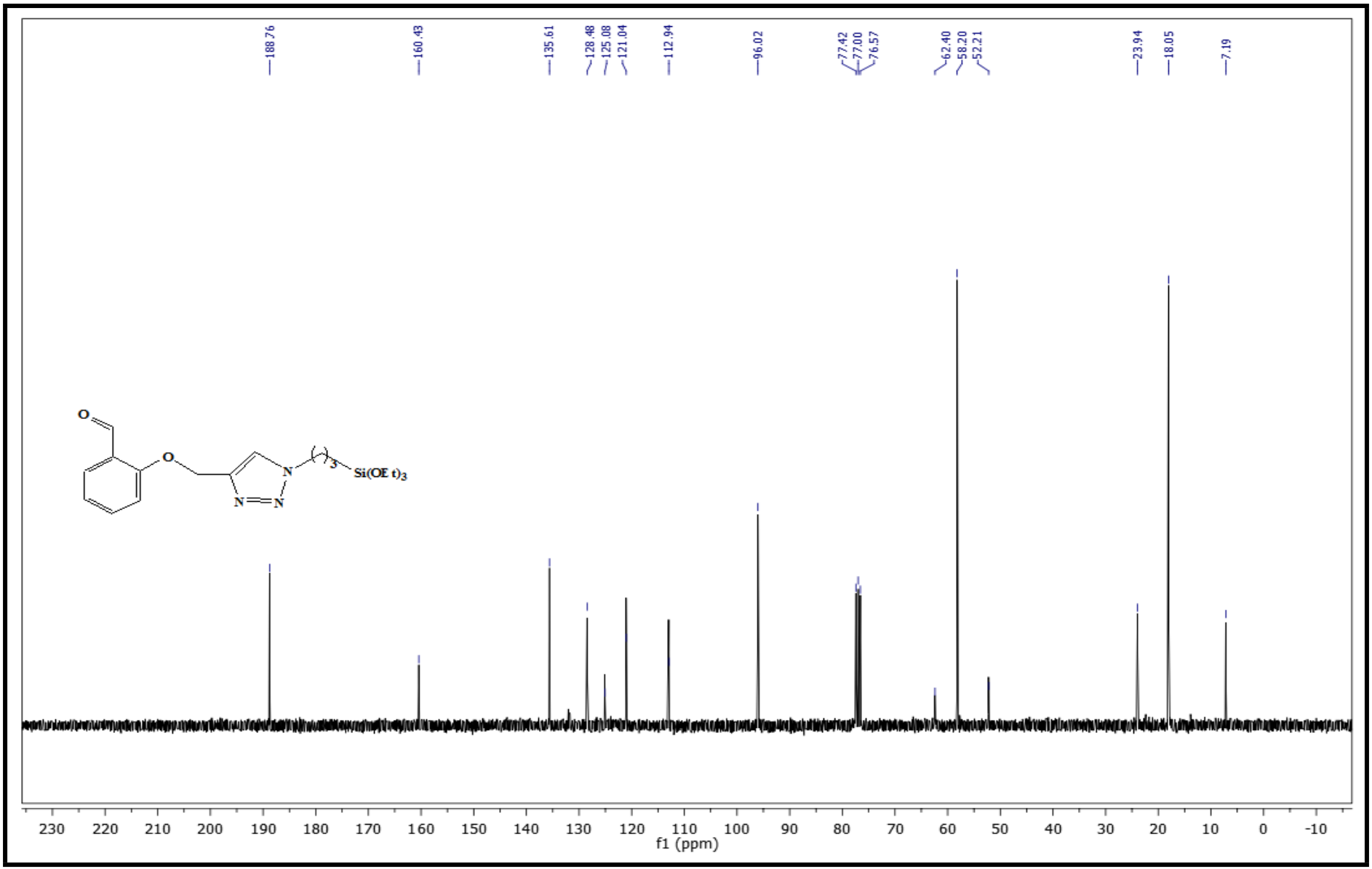
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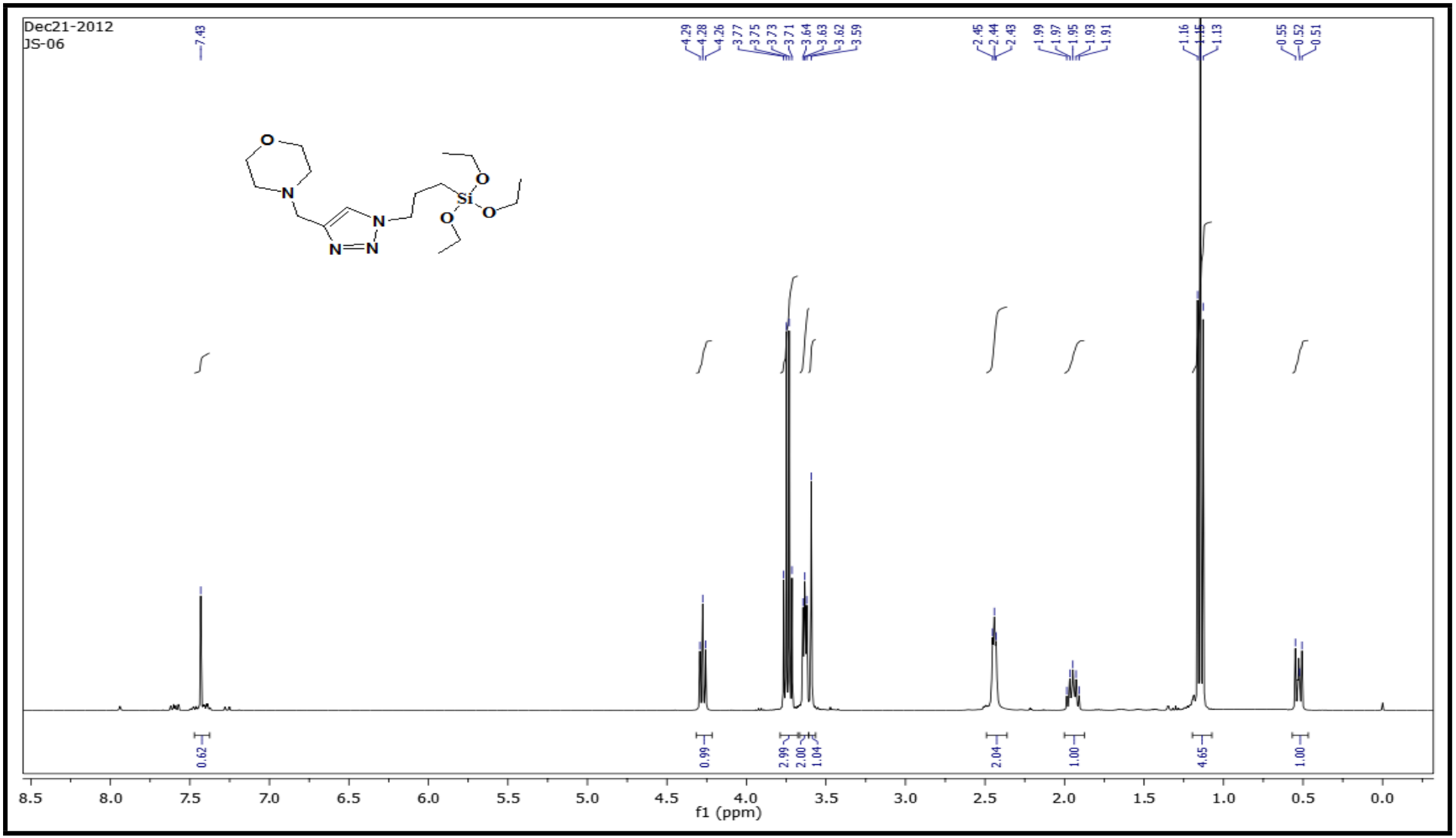
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O
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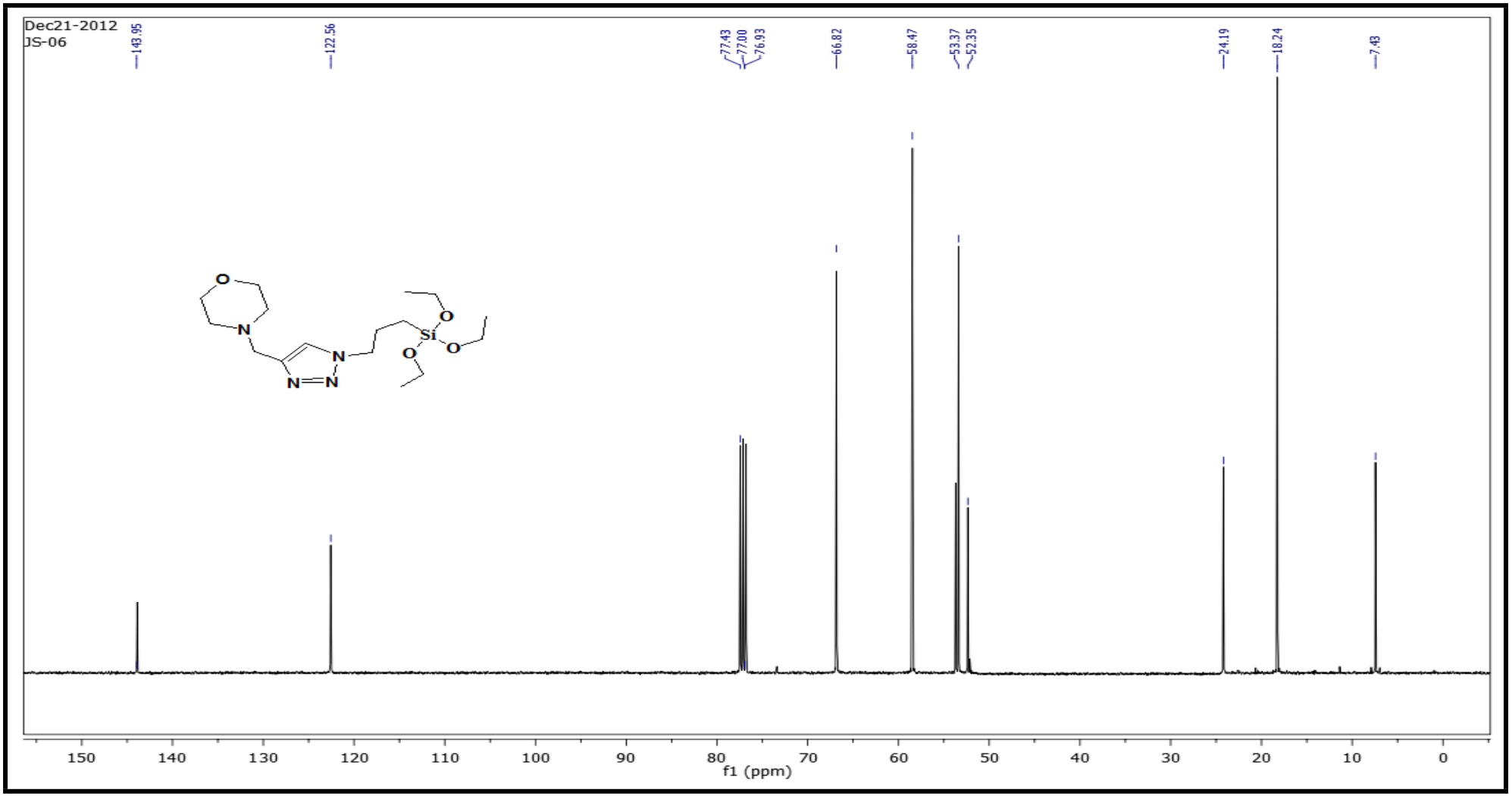
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Si
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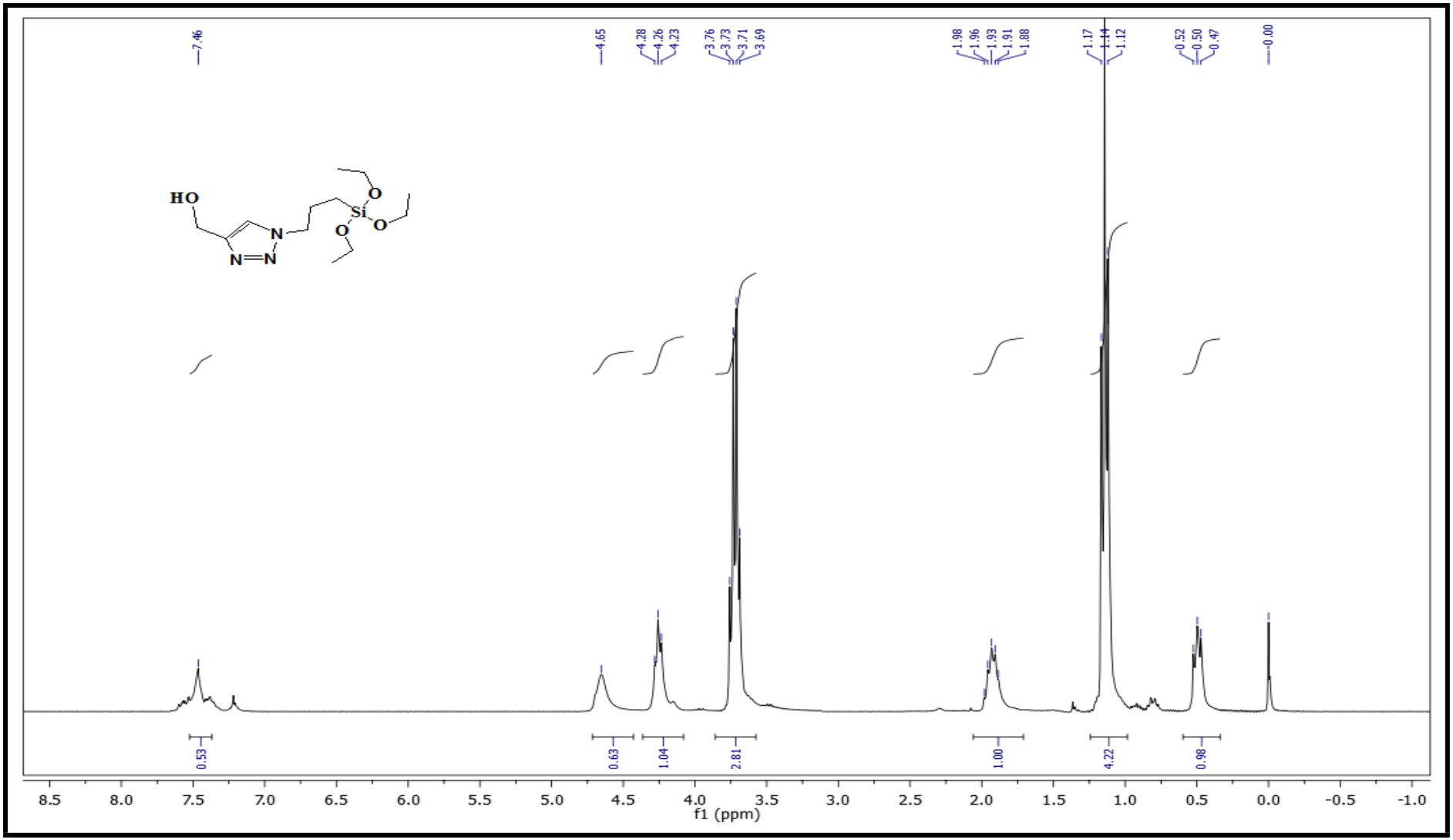
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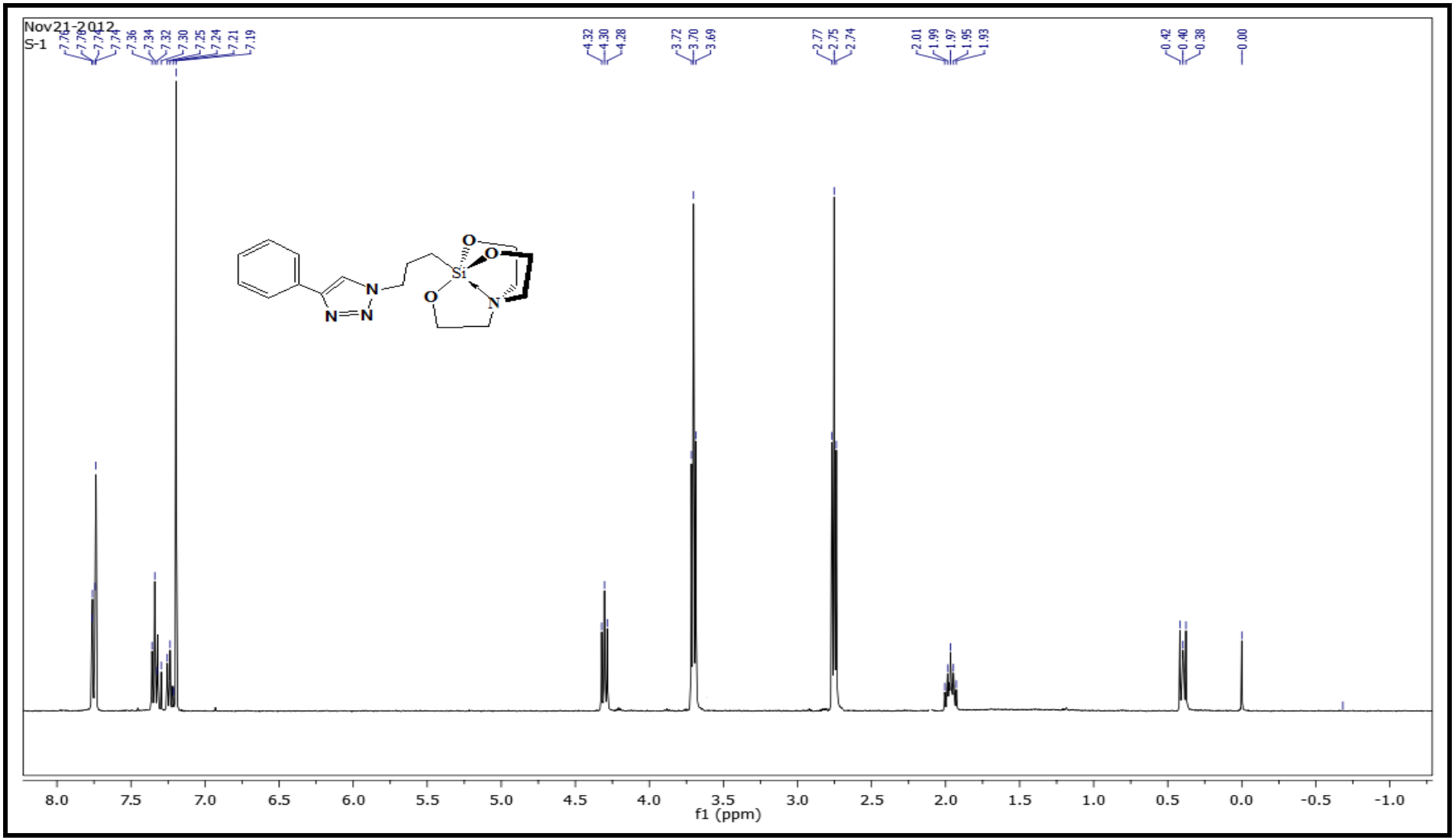
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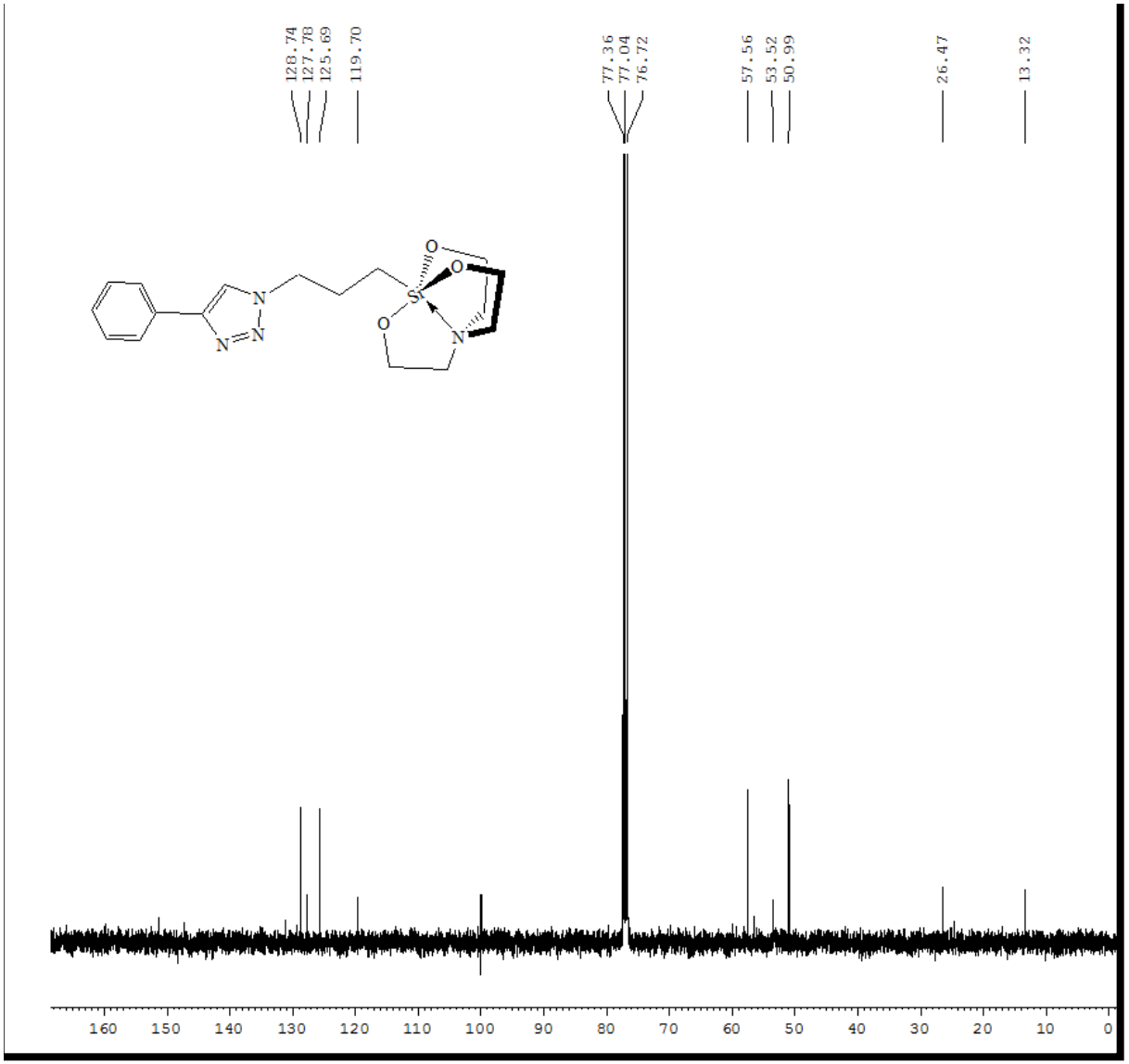
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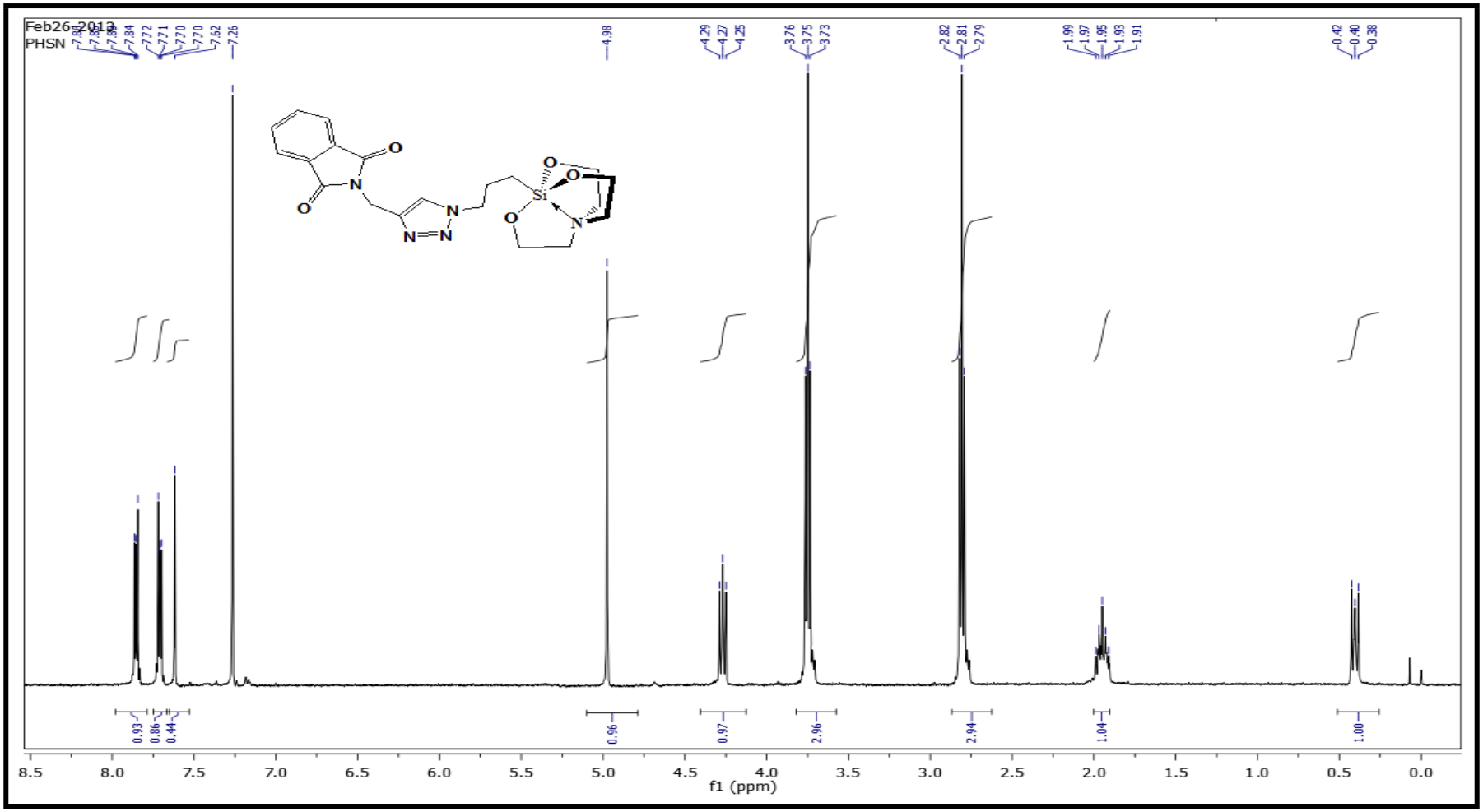
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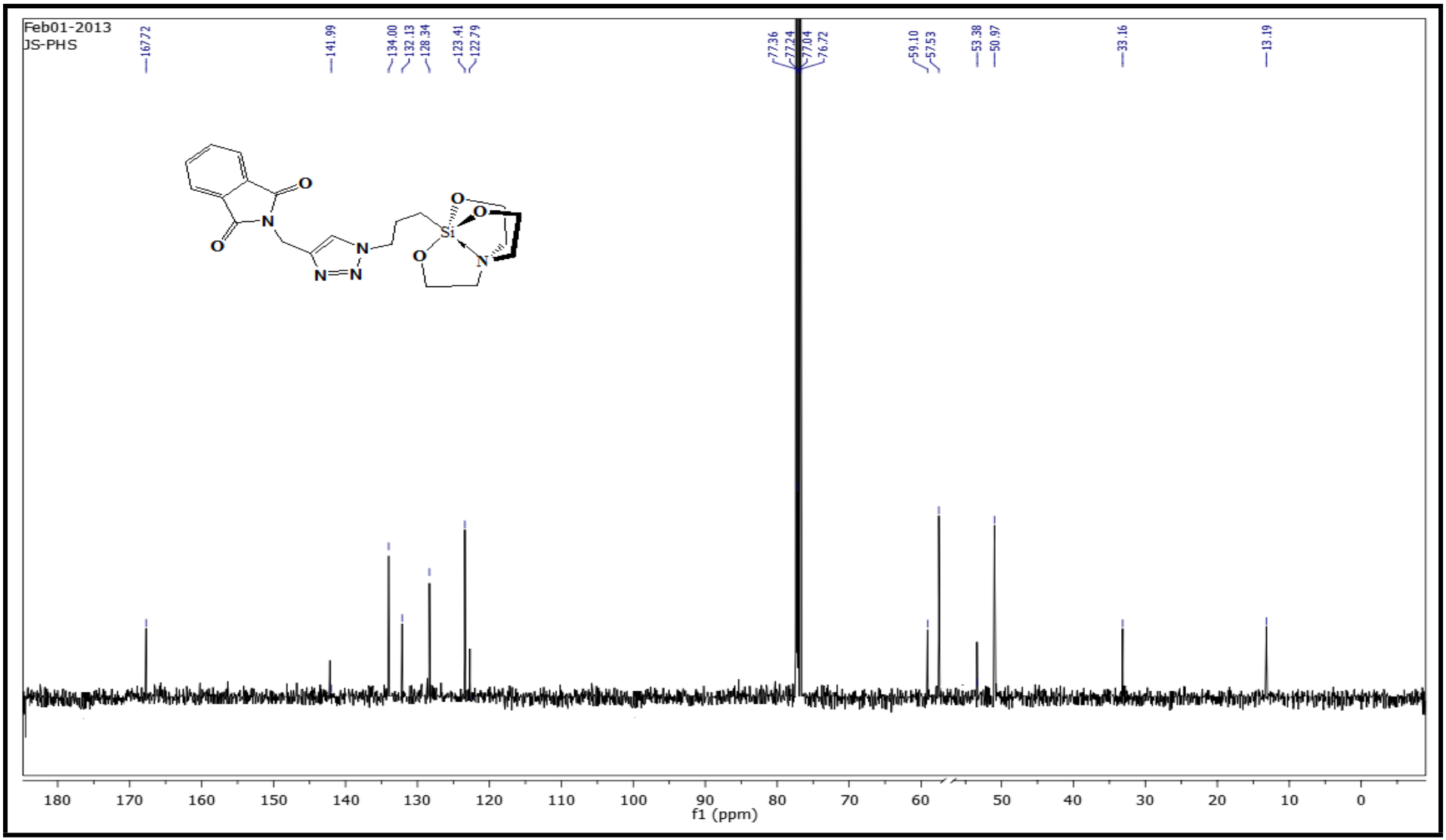
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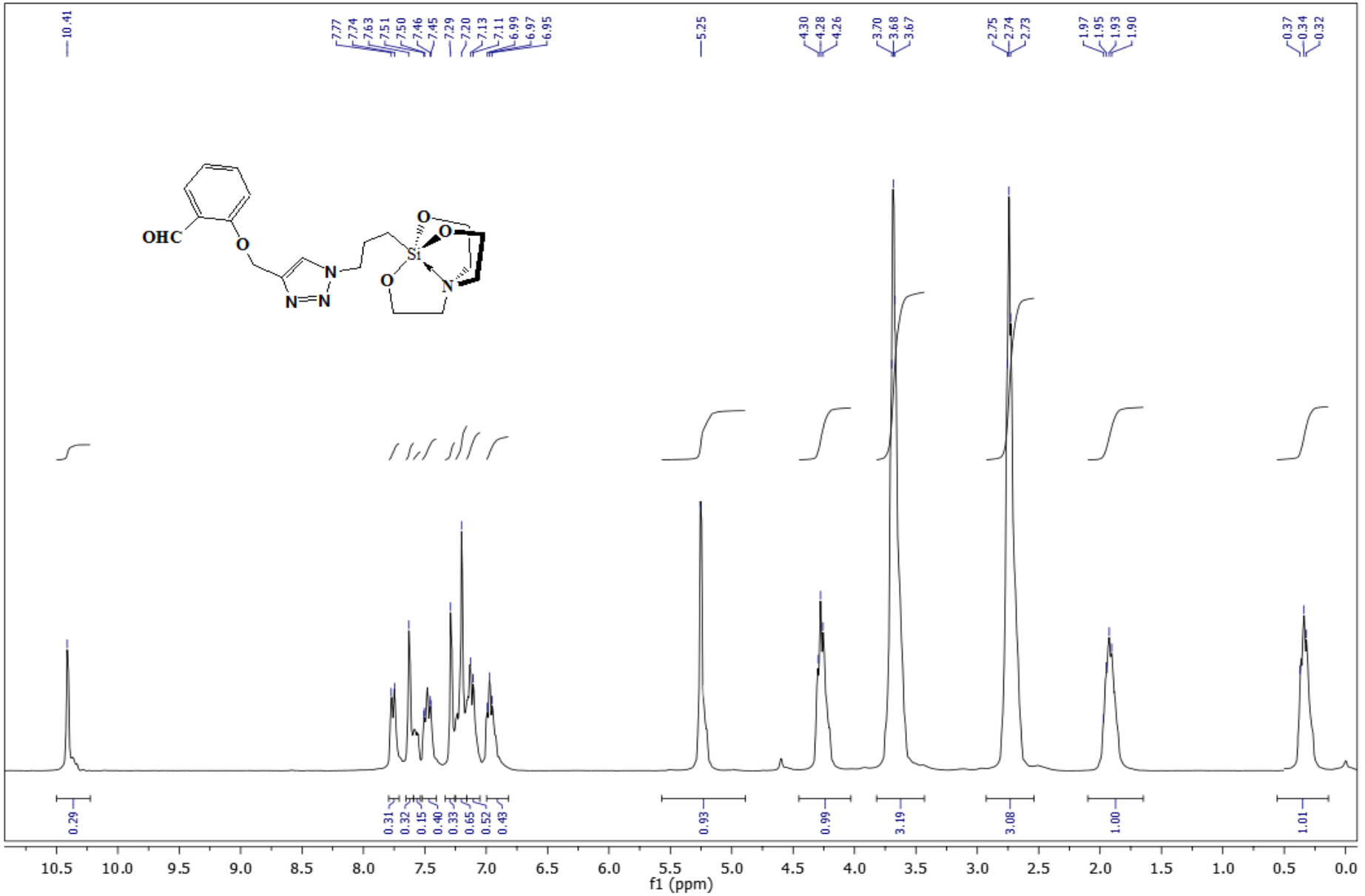
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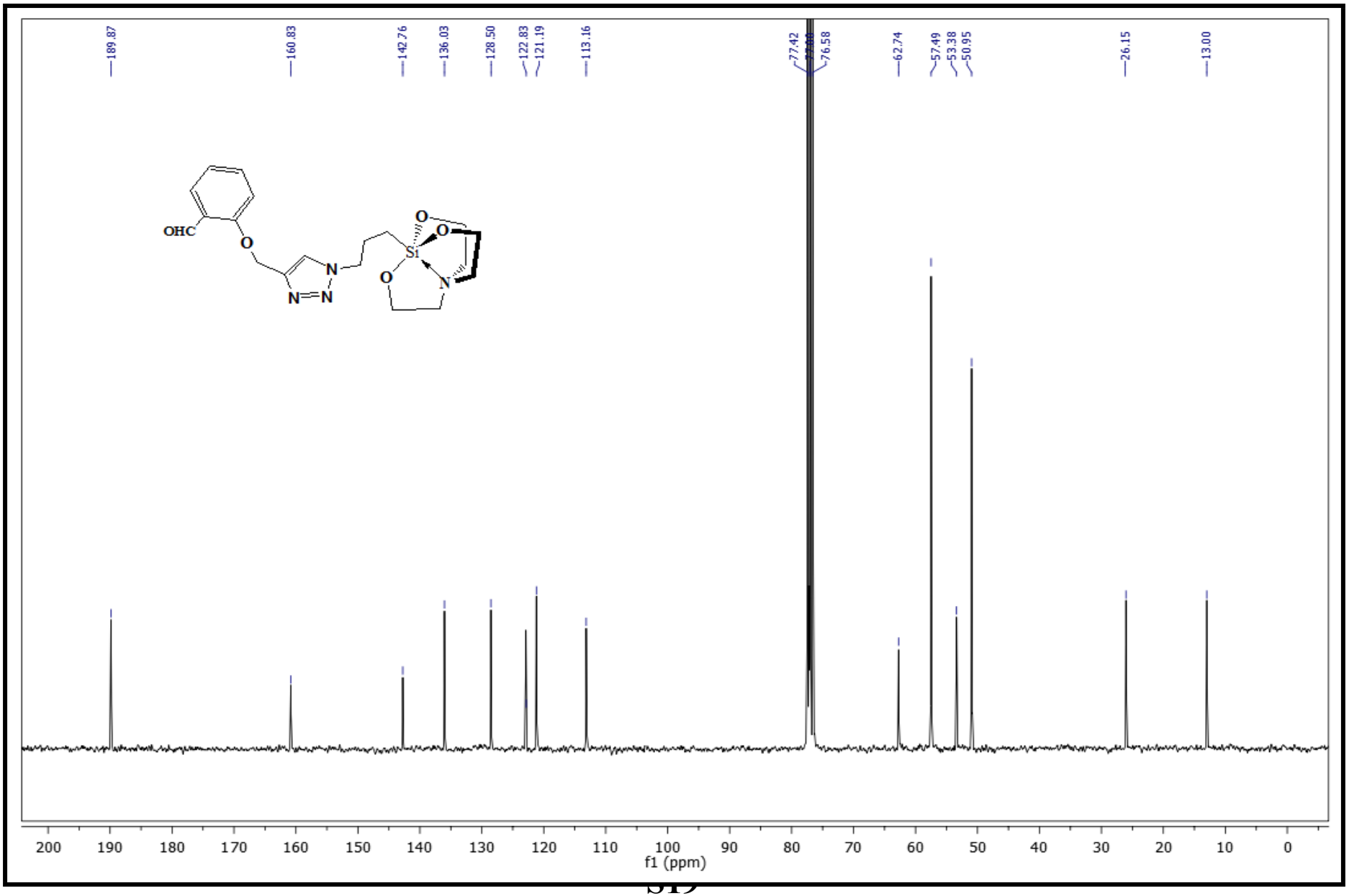
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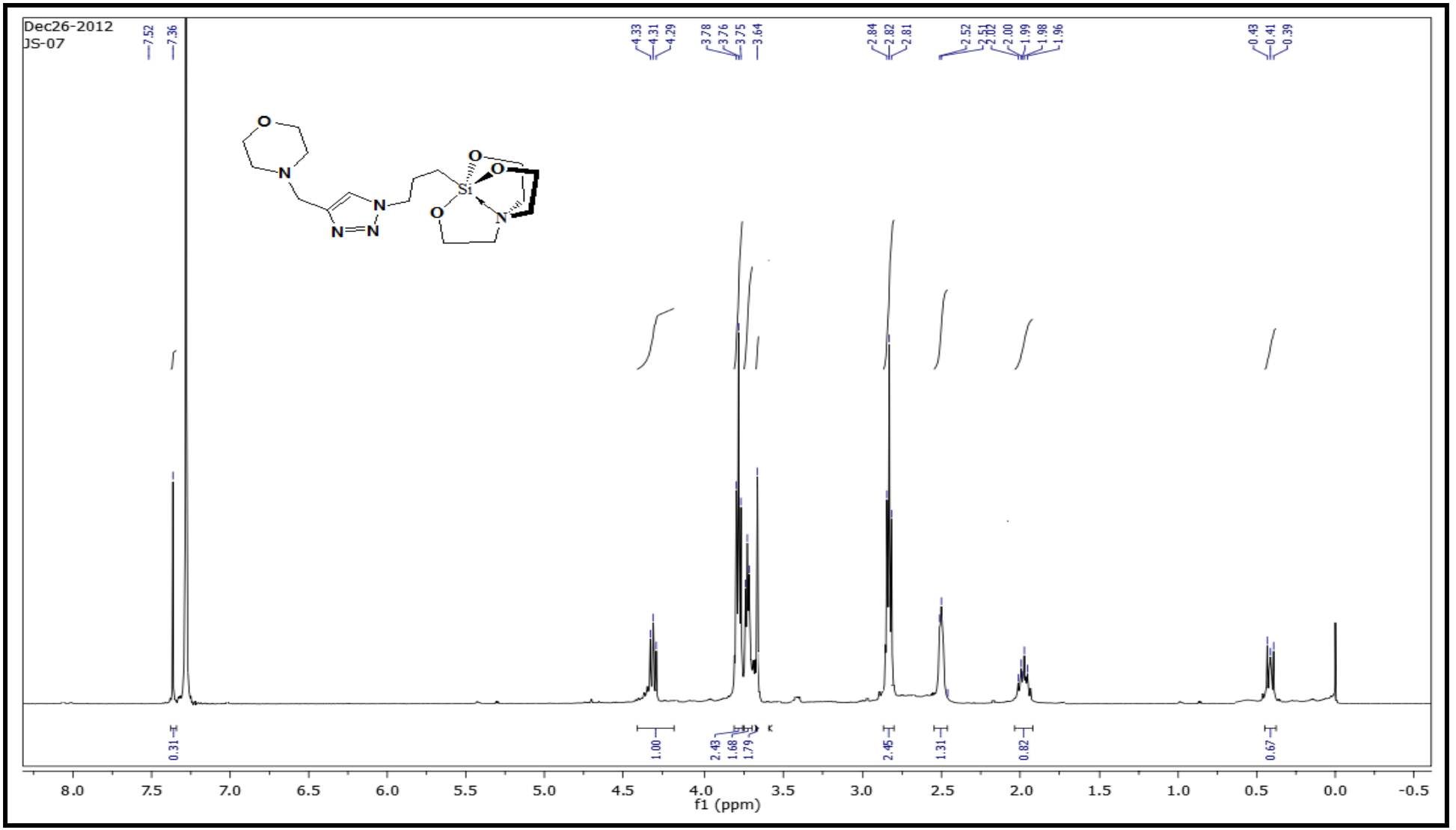
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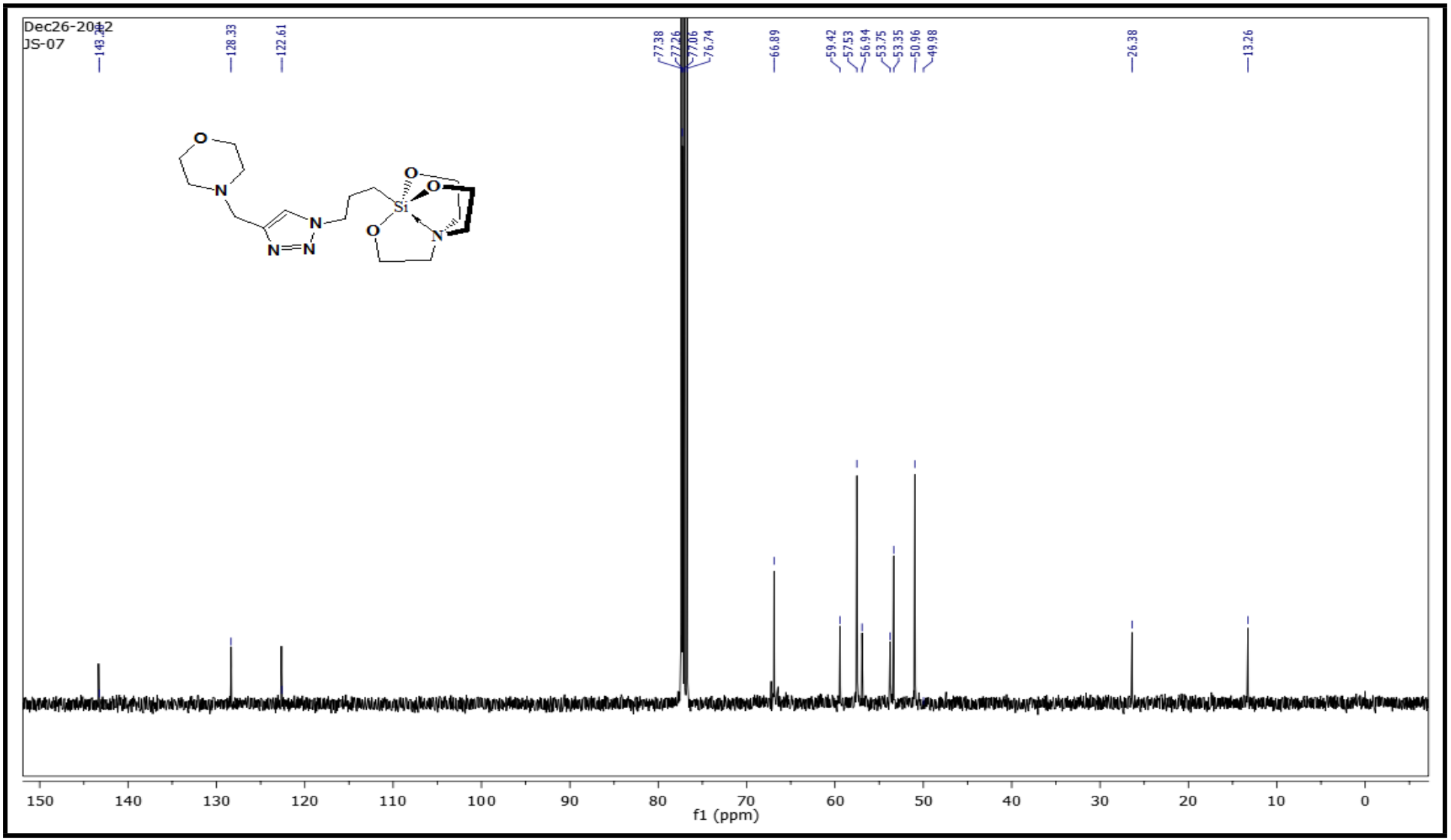
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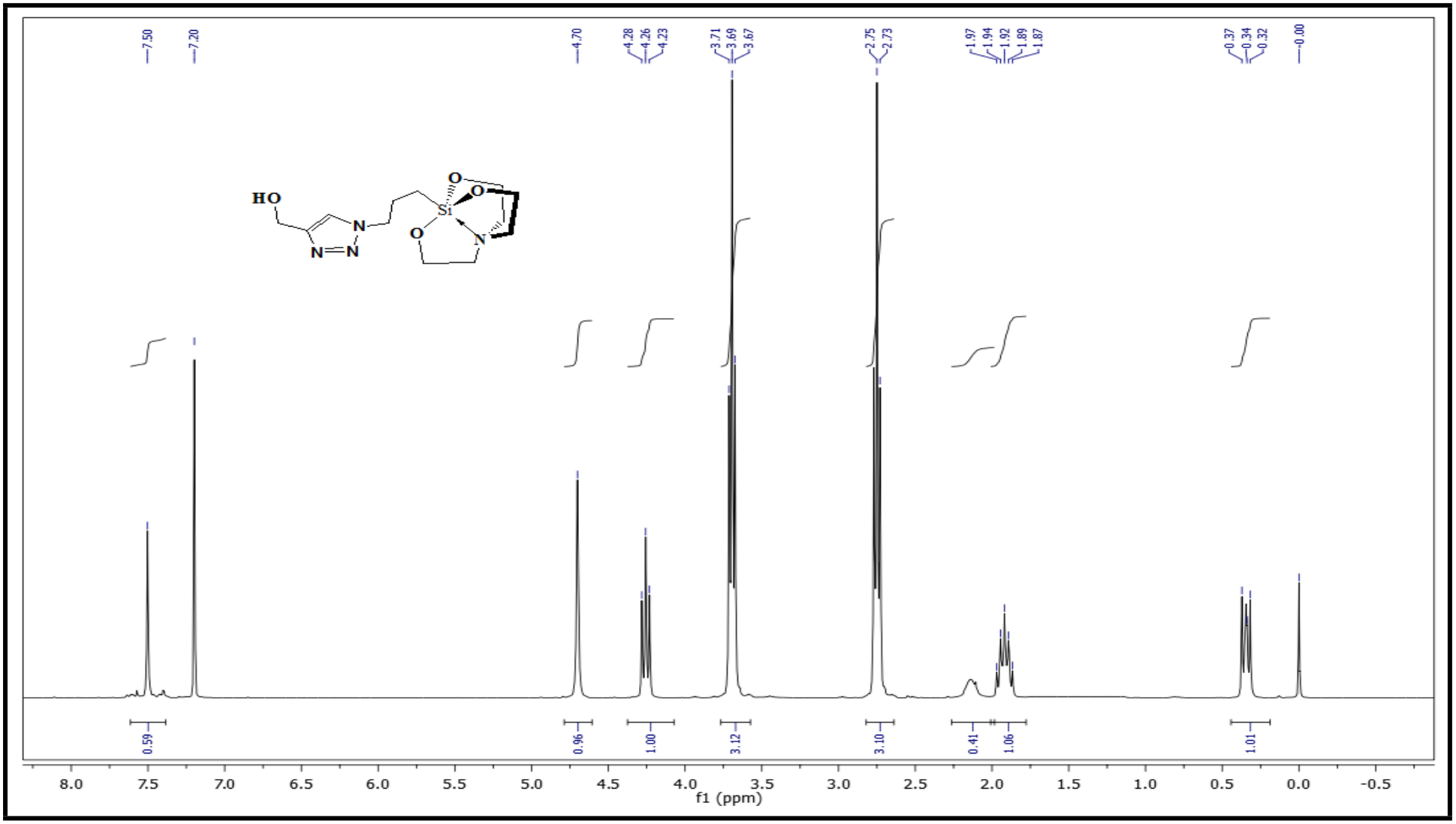
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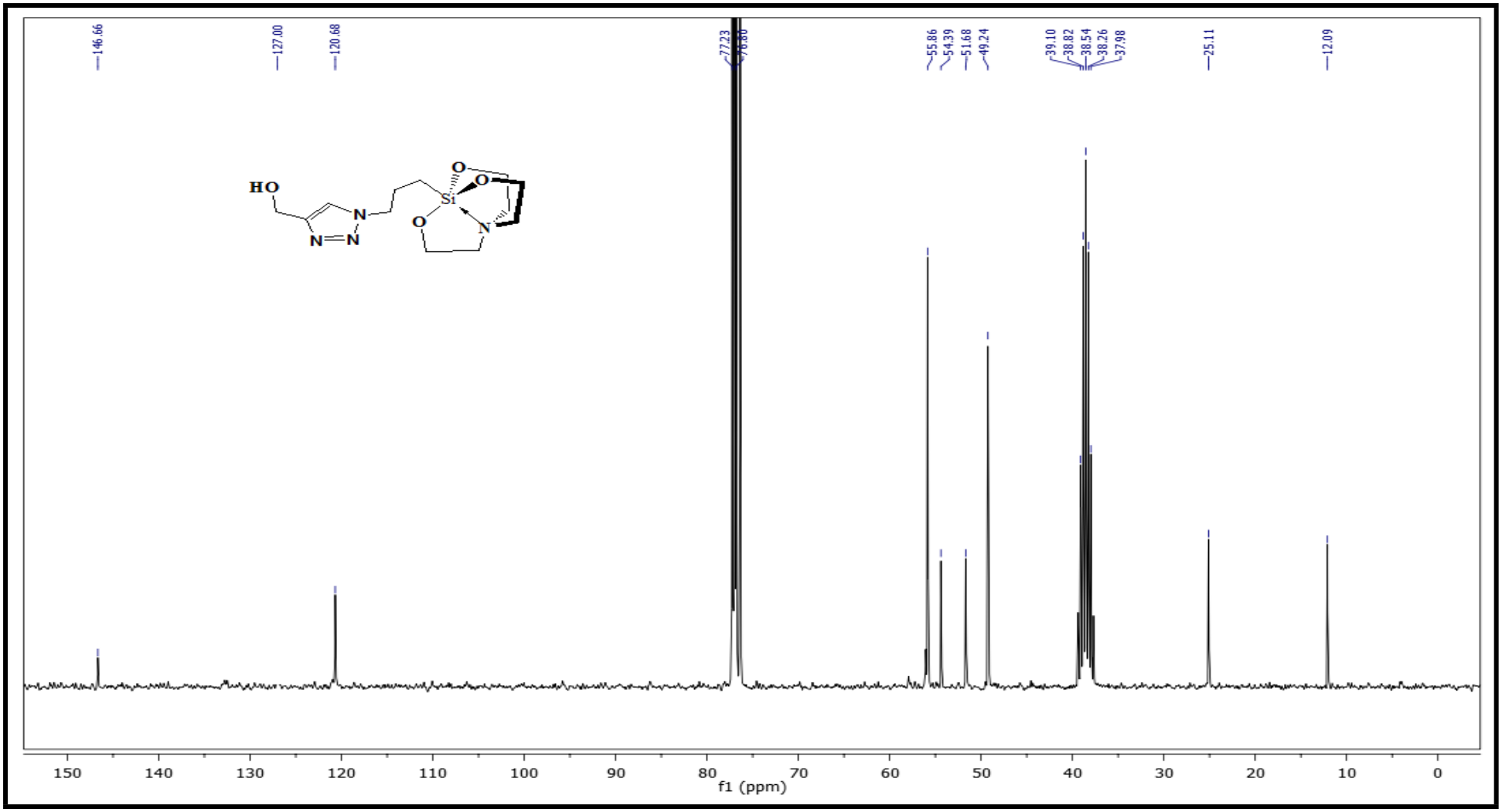
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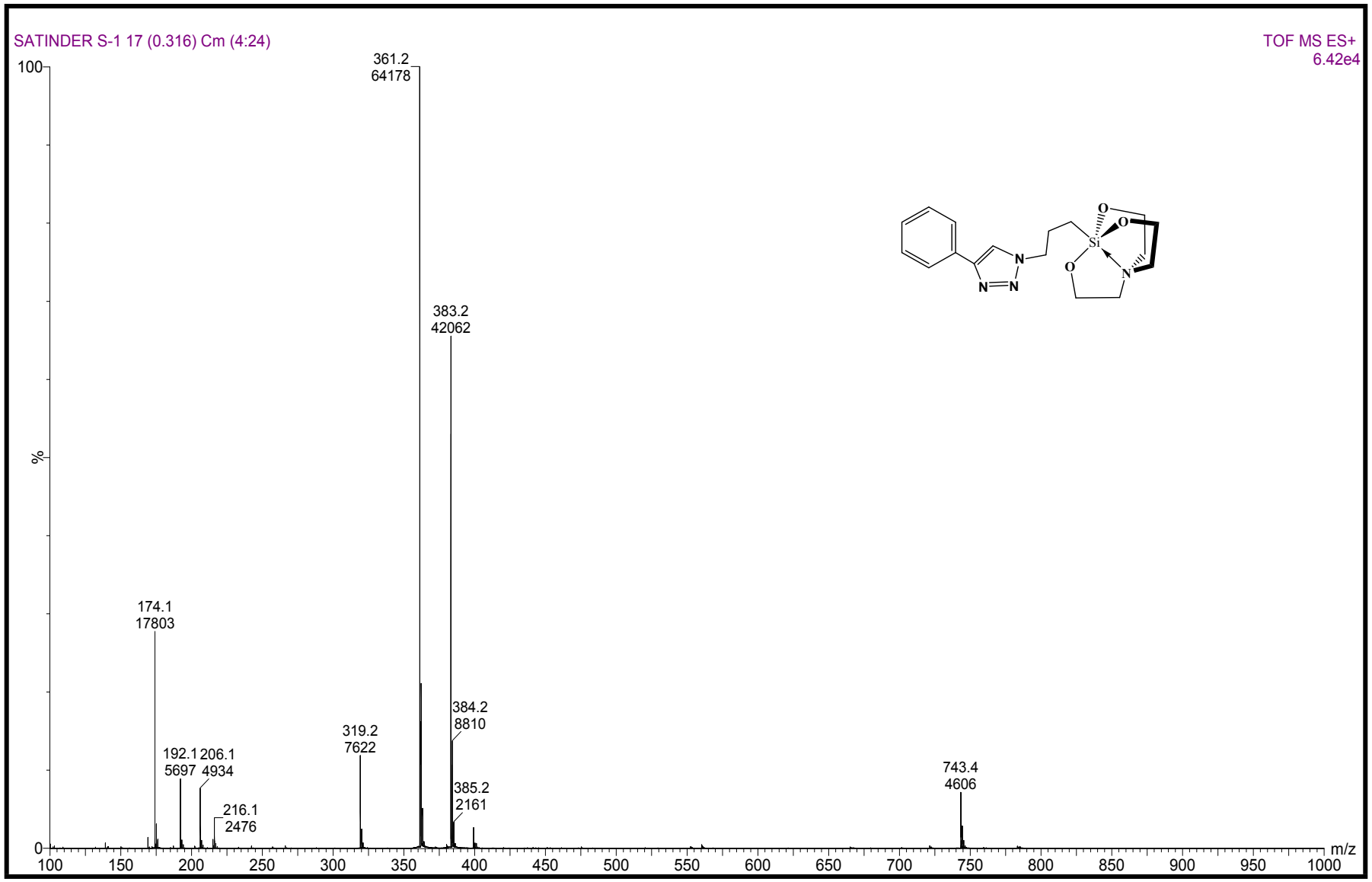
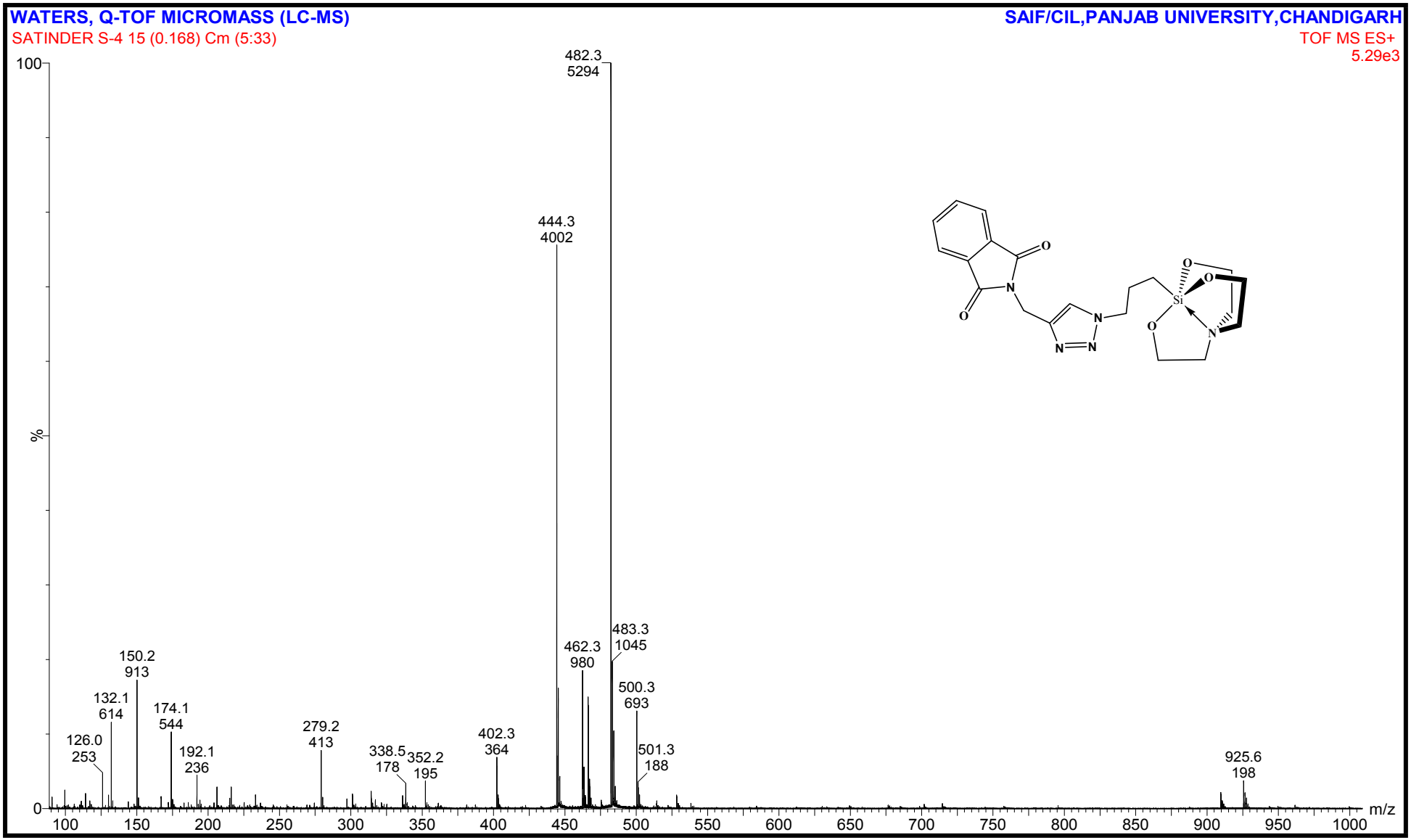
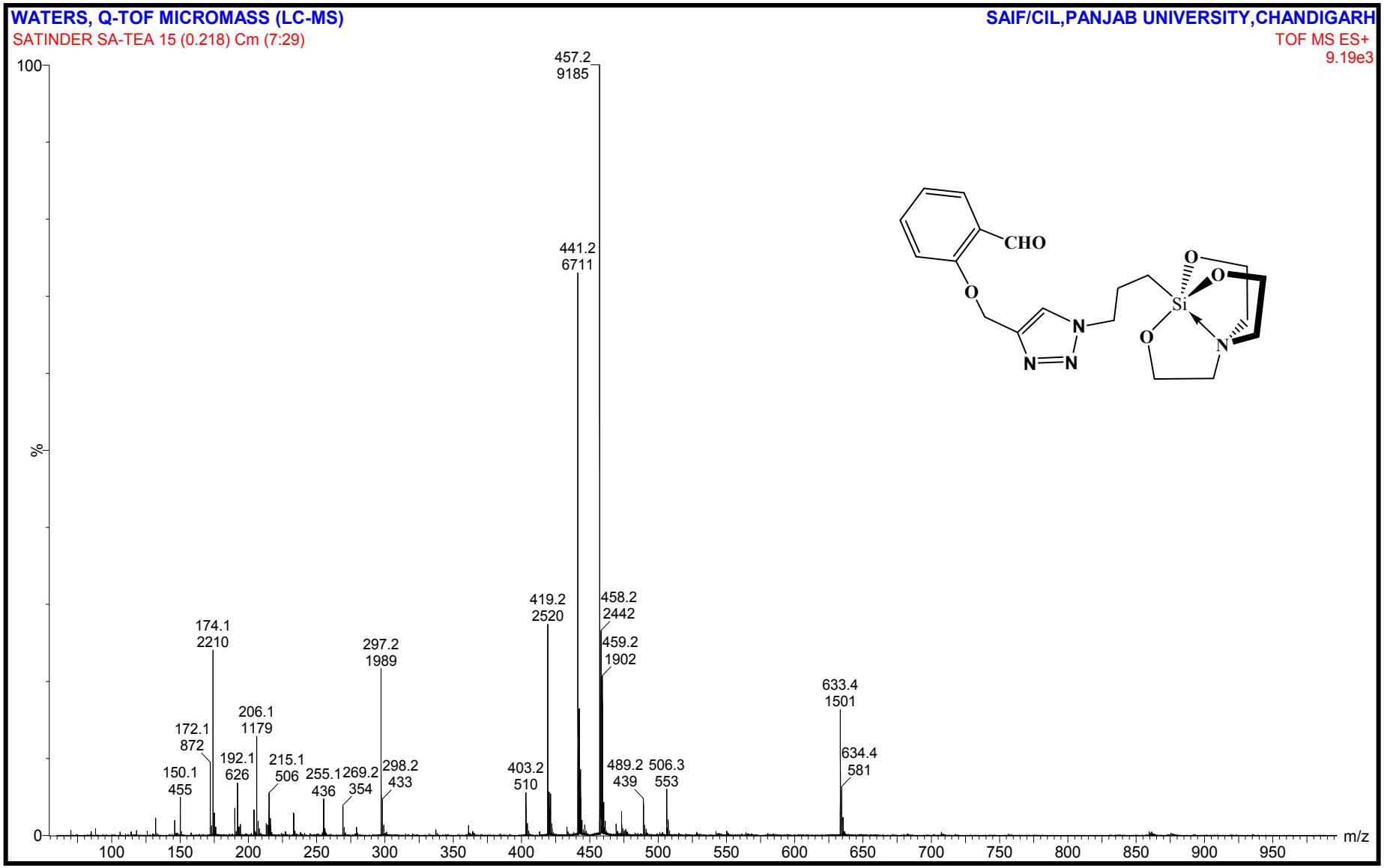
50
40
30
20
10
0
f1 (ppm)


SATINDER S-1 17 (0.316) Cm (4:24)
TOF MS ES+
6.42e4
100
%
0
361.2
64178
383.2
42062
174.1
17803
384.2
8810
319.2
7622
192.1
5697
206.1
4934
385.2
2161
216.1
2476
743.4
4606
m/z
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000


WATERS, Q-TOF MICROMASS (LC-MS)
SATINDER S-4 15 (0.168) Cm (5:33)
SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH
TOF MS ES+
5.29e3
100
%
0
m/z
482.3
5294
444.3
4002
462.3
980
483.3
1045
500.3
693
501.3
188
150.2
913
132.1
614
174.1
544
126.0
253
192.1
236
279.2
413
338.5
178
352.2
195
402.3
364
925.6
198
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000


WATERS, Q-TOF MICROMASS (LC-MS)
SATINDER SA-TEA 15 (0.218) Cm (7:29)
SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH
TOF MS ES+
9.19e3
100
%
0
457.2
9185
441.2
6711
419.2
2520
458.2
2442
459.2
1902
174.1
2210
297.2
1989
206.1
1179
172.1
872
192.1
626
215.1
506
255.1
436
269.2
354
298.2
433
150.1
455
403.2
510
489.2
439
506.3
553
633.4
1501
634.4
581
CHO
O
N
N
N
Si
O
O
O
O
N
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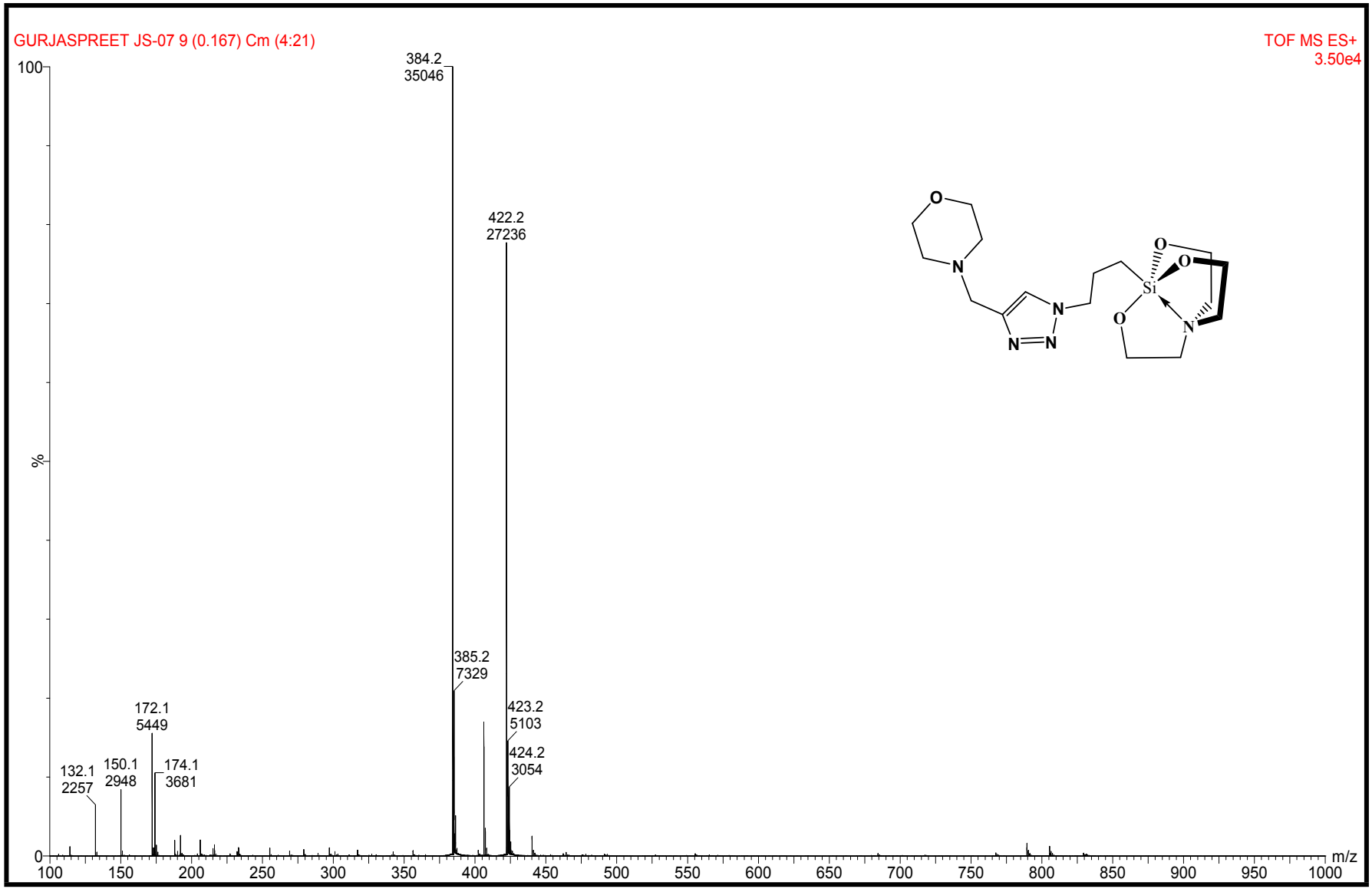
600
650
700
750
800
850
900
950
m/z


GURJASPREET JS-07 9 (0.167) Cm (4:21)
TOF MS ES+
3.50e4
100
%
0
384.2
35046
422.2
27236
385.2
7329
423.2
5103
424.2
3054
172.1
5449
132.1
2257
150.1
2948
174.1
3681
m/z
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
O
N
N
N
O
O
Si
O
N

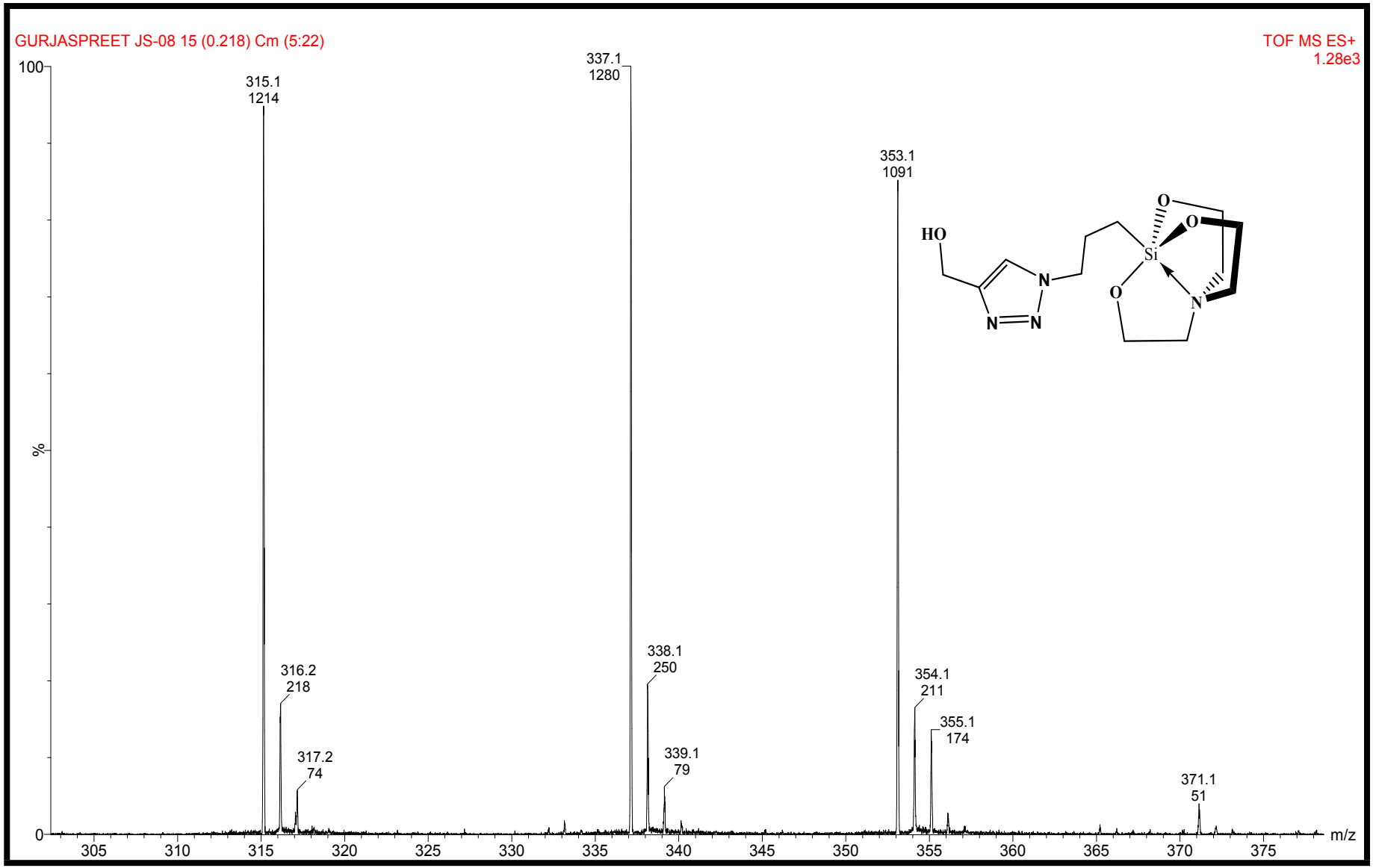

GURJASPREET JS-08 15 (0.218) Cm (5:22)
TOF MS ES+
1.28e3
100
%
0
315.1
1214
337.1
1280
353.1
1091
316.2
218
317.2
74
338.1
250
339.1
79
354.1
211
355.1
174
371.1
51
HO
N
N
N
Si
O
O
O
N
305
310
315
320
325
330
335
340
345
350
355
360
365
370
375
m/z

Table S1: Selected bond lengths (Å) and angles (°) of 1-(3-(silatranyl)propyl)-1H-1,2,3-triazol-4-yl)benzene **(2a)**

Parameter	X-ray crystal data	Parameter	X-ray crystal data
C(7)-N(1)	1.362(3)	C(5)-C(6)-C(1)	120.6(3)
C(7)-C(8)	1.382(4)	N(1)-C(7)-C(8)	108.0(2)
C(8)-N(3)	1.344(3)	N(1)-C(7)-C(4)	121.4(2)
C(9)-N(3)	1.468(3)	C(8)-C(7)-C(4)	130.6(2)
C(11)-Si(1)	1.882(3)	N(3)-C(8)-C(7)	104.7(2)
C(12)-O(3)	1.398(4)	N(3)-C(9)-C(10)	112.5(2)
C(13)-N(4)	1.469(4)	C(9)-C(10)-C(11)	114.6(2)
C(14)-O(2)	1.427(3)	C(10)-C(11)-Si(1)	116.9(2)
C(14)-C(15)	1.517(4)	O(3)-C(12)-C(13)	109.7(2)
C(15)-N(4)	1.474(3)	N(4)-C(13)-C(12)	106.1(2)
C(16)-O(1)	1.421(3)	O(2)-C(14)-C(15)	108.3(2)
C(17)-N(4)	1.475(3)	N(4)-C(15)-C(14)	106.2(2)
N(1)-N(2)	1.319(3)	O(1)-C(16)-C(17)	109.1(2)
N(2)-N(3)	1.343(3)	N(4)-C(17)-C(16)	106.4(2)
N(4)-Si(1)	2.156(3)	O(2)-C(14)-C(15)	108.3(2)
O(1)-Si(1)	1.6719(19)	N(4)-C(15)-C(14)	106.2(2)
O(2)-Si(1)	1.6673(19)	O(1)-C(16)-C(17)	109.1(2)
O(3)-Si(1)	1.670(2)	N(4)-C(17)-C(16)	106.4(2)
C(13)-N(4)-C(17)	114.0(2)	N(2)-N(1)-C(7)	108.9(2)
C(15)-N(4)-C(17)	114.5(2)	N(1)-N(2)-N(3)	107.2(2)

C(13)-N(4)-Si(1)	104.90(18)	N(2)-N(3)-C(8)	111.2(2)
C(15)-N(4)-Si(1)	103.62(17)	C(8)-N(3)-C(9)	129.5(2)
C(17)-N(4)-Si(1)	104.33(16)	C(13)-N(4)-C(15)	113.9(2)
C(16)-O(1)-Si(1)	123.14(18)	O(2)-Si(1)-O(3)	118.30(11)
C(14)-O(2)-Si(1)	122.04(17)	O(2)-Si(1)-O(1)	117.89(11)
C(12)-O(3)-Si(1)	123.8(2)	O(2)-Si(1)-C(11)	98.74(11)
O(2)-Si(1)-O(3)	118.30(11)	O(3)-Si(1)-C(11)	96.34(13)
O(2)-Si(1)-O(1)	117.89(11)	O(1)-Si(1)-C(11)	94.80(11)
O(3)-Si(1)-O(1)	119.89(11)	O(2)-Si(1)-N(4)	83.86(9)
O(2)-Si(1)-C(11)	98.74(11)	O(3)-Si(1)-N(4)	82.90(11)
O(3)-Si(1)-C(11)	96.34(13)	C(11)-Si(1)-N(4)	177.32(11)

Table S2: Selected bond lengths (Å) and angles (°) of N-((1-(3-(silatranyl)propyl)-1H-1,2,3-triazol-4-yl)methyl)phthalimide (**2b**)

Parameter	X-ray crystal data	Parameter	X-ray crystal data
C(8)-O(2)	1.212(2)	N(2)-C(10)-C(11)	108.18(18)
C(8)-N(1)	1.395(3)	N(2)-C(10)-C(9)	122.11(17)
C(9)-N(1)	1.457(2)	C(11)-C(10)-C(9)	129.67(18)
C(10)-N(2)	1.359(3)	N(4)-C(11)-C(10)	105.38(18)
C(11)-N(4)	1.342(3)	N(4)-C(12)-C(13)	109.95(16)
C(12)-N(4)	1.465(2)	C(12)-C(13)-C(14)	113.08(17)
C(12)-C(13)	1.526(3)	C(13)-C(14)-Si(1)	114.18(14)
C(13)-C(14)	1.533(3)	O(3)-C(15)-C(16)	108.30(18)
C(14)-Si(1)	1.884(2)	N(5)-C(16)-C(15)	106.27(19)
C(15)-O(3)	1.417(3)	O(4)-C(17)-C(18)	109.08(18)
C(15)-C(16)	1.518(3)	N(5)-C(18)-C(17)	105.86(17)
C(16)-N(5)	1.476(3)	O(5)-C(19)-C(20)	108.8(2)
C(17)-O(4)	1.424(3)	N(5)-C(20)-C(19)	106.21(19)
C(17)-C(18)	1.512(3)	C(7)-N(1)-C(8)	112.31(16)
C(18)-N(5)	1.471(3)	C(7)-N(1)-C(9)	124.26(17)
C(19)-O(5)	1.426(3)	C(8)-N(1)-C(9)	123.43(16)
C(19)-C(20)	1.511(4)	N(3)-N(2)-C(10)	108.81(16)
C(20)-N(5)	1.471(3)	N(2)-N(3)-N(4)	107.05(16)
N(2)-N(3)	1.319(2)	C(11)-N(4)-N(3)	110.57(16)
N(3)-N(4)	1.347(2)	C(11)-N(4)-C(12)	128.90(17)

N(5)-Si(1)	2.1847(18)	N(3)-N(4)-C(12)	119.75(16)
O(3)-Si(1)	1.6745(15)	C(18)-N(5)-C(20)	114.33(18)
O(4)-Si(1)	1.6625(16)	C(18)-N(5)-C(16)	113.18(18)
O(5)-Si(1)	1.6653(16)	C(20)-N(5)-C(16)	114.00(19)
N(1)-C(9)-C(10)	113.31(16)	C(18)-N(5)-Si(1)	104.72(13)
C(17)-O(4)-Si(1)	122.14(13)	C(20)-N(5)-Si(1)	104.62(13)
C(15)-O(3)-Si(1)	122.87(14)	C(16)-N(5)-Si(1)	104.59(13)
C(19)-O(5)-Si(1)	122.25(14)	O(5)-Si(1)-O(3)	118.41(9)
O(4)-Si(1)-O(5)	119.08(9)117.87(8)	O(4)-Si(1)-C(14)	98.33(9)
O(4)-Si(1)-O(3)	178.53(9)	O(5)-Si(1)-C(14)	97.10(9)
C(14)-Si(1)-N(5)		O(4)-Si(1)-N(5)	82.93(7)

Table S3: Selected bond lengths (Å) and angles (°) of N-((1-(3-(silatranyl)propyl)-1H-1,2,3-triazol-4-yl)methyl)morpholine (**2d**)

Parameter	X-ray crystal data	Parameter	X-ray crystal data
C(5)-N(1)	1.471(3)	C(1)-N(1)-C(4)	108.8(2)
C(5)-C(6)	1.488(4)	C(1)-N(1)-C(5)	112.09(19)
C(6)-N(2)	1.356(3)	C(4)-N(1)-C(5)	111.2(2)
C(6)-C(7)	1.373(3)	N(3)-N(2)-C(6)	109.0(2)
C(7)-N(4)	1.350(3)	N(2)-N(3)-N(4)	107.2(2)
C(8)-N(4)	1.465(3)	N(3)-N(4)-C(7)	110.5(2)
C(15)-N(5)	1.477(3)	N(3)-N(4)-C(8)	120.6(2)
C(15)-C(16)	1.518(3)	C(7)-N(4)-C(8)	128.7(2)
C(13)-O(3)	1.426(3)	C(14)-N(5)-C(15)	113.66(19)
C(14)-N(5)	1.475(3)	C(14)-N(5)-C(12)	113.35(18)
C(10)-Si(1)	1.889(3)	C(15)-N(5)-C(12)	113.6(2)
C(16)-O(4)	1.432(3)	C(14)-N(5)-Si(1)	105.13(15)
C(12)-N(5)	1.480(3)	C(15)-N(5)-Si(1)	104.81(14)
C(11)-O(2)	1.431(3)	C(12)-N(5)-Si(1)	105.07(14)
N(2)-N(3)	1.324(3)	C(16)-O(4)-Si(1)	122.38(14)
N(3)-N(4)	1.344(3)	C(11)-O(2)-Si(1)	122.63(14)
N(5)-Si(1)	2.134(2)	C(13)-O(3)-Si(1)	122.25(16)
O(4)-Si(1)	1.6703(18)	C(3)-O(1)-C(2)	110.4(2)
O(2)-Si(1)	1.6685(17)	O(2)-Si(1)-O(4)	119.81(9)
O(3)-Si(1)	1.6734(18)	O(2)-Si(1)-O(3)	118.92(9)

O(1)-C(2)-C(1)	110.6(2)	O(4)-Si(1)-O(3)	117.66(9)
O(1)-C(3)-C(4)	112.1(2)	O(2)-Si(1)-C(10)	95.79(10)
N(1)-C(4)-C(3)	110.4(2)	O(4)-Si(1)-C(10)	95.70(9)
N(1)-C(5)-C(6)	111.8(2)	O(3)-Si(1)-C(10)	97.55(11)
N(2)-C(6)-C(7)	108.0(2)	O(2)-Si(1)-N(5)	83.53(8)
N(2)-C(6)-C(5)	123.4(2)	C(10)-Si(1)-N(5)	178.75(10)
C(7)-C(6)-C(5)	128.6(2)	N(5)-C(12)-C(11)	105.66(18)
N(4)-C(7)-C(6)	105.3(2)	O(3)-C(13)-C(14)	109.18(19)
N(4)-C(8)-C(9)	111.94(19)	N(5)-C(14)-C(13)	106.12(19)
N(5)-C(15)-C(16)	105.8(2)	C(8)-C(9)-C(10)	112.51(19)
O(4)-C(16)-C(15)	108.59(19)	C(9)-C(10)-Si(1)	115.14(16)

Table S4: Selected bond lengths (Å) and angles (°) of (1-(3-(silatranyl)propyl)-1H-1,2,3-triazol-4-yl)methanol (**2e**)

Parameter	X-ray crystal data	Parameter	X-ray crystal data
N(4)-Si(1)	2.146(2)	O(1)-C(1)-C(2)	112.6(2)
N(1)-N(2)	1.314(3)	N(1)-C(2)-C(3)	107.0(2)
N(2)-N(3)	1.336(3)	N(1)-C(2)-C(1)	121.6(2)
O(2)-Si(1)	1.6741(19)	C(4)-C(5)-C(6)	109.9(2)
O(3)-Si(1)	1.6591(19)	C(5)-C(6)-Si(1)	118.42(18)
O(4)-Si(1)	1.6644(19)	O(4)-C(7)-C(8)	108.0(2)
C(6)-Si(1)	1.876(2)	O(3)-C(9)-C(10)	108.6(2)
C(4)-N(3)	1.470(3)	O(2)-C(11)-C(12)	108.8(2)
C(10)-N(4)	1.458(4)	N(4)-C(10)-C(9)	106.6(2)
C(12)-N(4)	1.479(4)	N(4)-C(8)-C(7)	105.6(2)
C(8)-N(4)	1.478(3)	N(4)-C(12)-C(11)	107.3(2)
C(2)-N(1)	1.347(4)	N(2)-N(1)-C(2)	109.7(2)
C(3)-N(3)	1.337(3)	N(1)-N(2)-N(3)	107.2(2)
C(2)-C(3)	1.374(3)	N(2)-N(3)-C(3)	110.2(2)
O(1)-H(1O)	1.01(5)	N(2)-N(3)-C(4)	118.5(2)
C(1)-O(1)	1.419(3)	C(3)-N(3)-C(4)	131.3(2)
C(1)-C(2)	1.485(4)	C(10)-N(4)-C(8)	114.6(2)
C(7)-O(4)	1.425(3)	C(10)-N(4)-C(12)	113.9(2)
C(9)-O(3)	1.420(3)	C(8)-N(4)-C(12)	112.3(2)
C(11)-O(2)	1.435(3)	C(10)-N(4)-Si(1)	104.81(16)

C(8)-N(4)-Si(1)	105.24(16)	C(9)-O(3)-Si(1)	123.04(18)
C(12)-N(4)-Si(1)	104.69(15)	C(7)-O(4)-Si(1)	122.53(18)
C(1)-O(1)-H(1O)	107(3)	O(3)-Si(1)-O(4)	122.75(12)
C(11)-O(2)-Si(1)	122.11(17)	O(3)-Si(1)-O(2)	116.58(11)
O(3)-Si(1)-N(4)	83.53(9)	O(4)-Si(1)-O(2)	116.90(12)
O(4)-Si(1)-N(4)	83.17(9)	O(3)-Si(1)-C(6)	96.58(11)
O(2)-Si(1)-N(4)	83.90(9)	O(4)-Si(1)-C(6)	94.78(10)
C(6)-Si(1)-N(4)	177.60(10)	O(2)-Si(1)-C(6)	98.17(10)

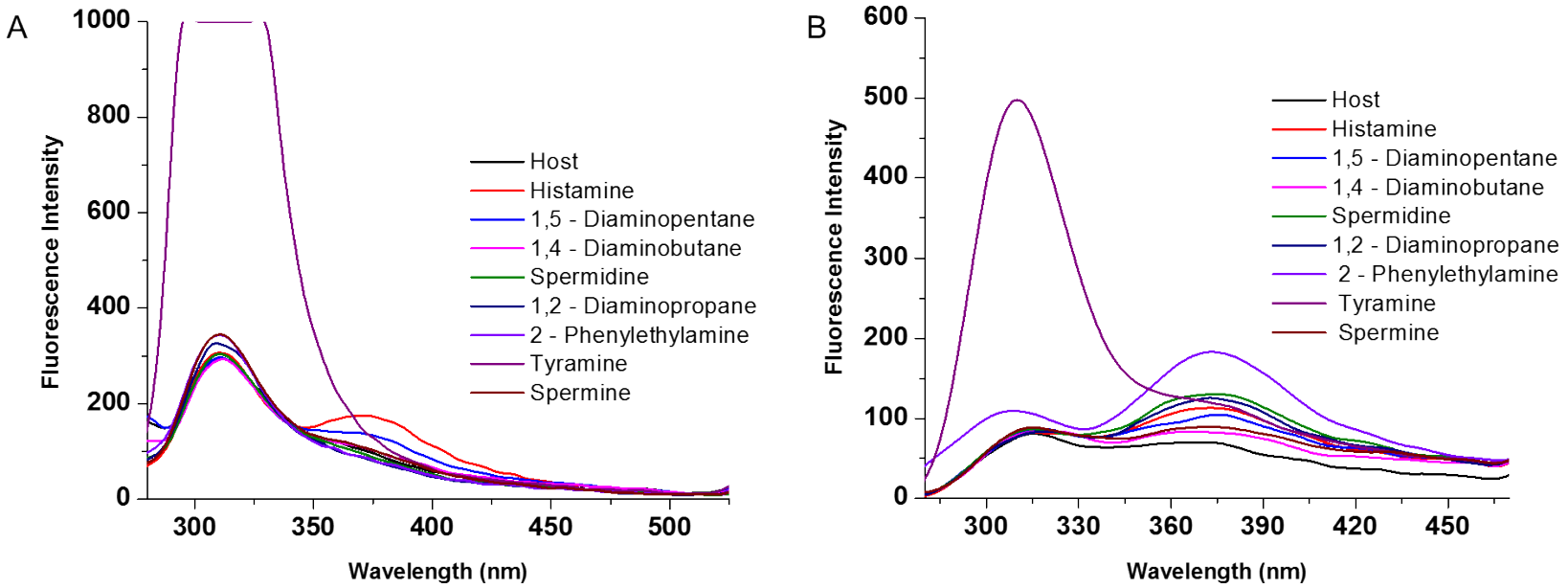


Figure S1: (A) Change in fluorescence intensity of **2a** upon addition various biogenic amines (histamine, spermine, spermidine, tryamine, 1,2-Diaminopropane, 1,4-Diaminobutane, 1,5-Diaminopentane, 2-Phenylethylamine) in CH_3CN/H_2O (98:2; v/v) solvent system; (B) Change in fluorescence intensity of **2b** upon addition various biogenic amines in CH_3CN/H_2O (98:2; v/v) solvent system.

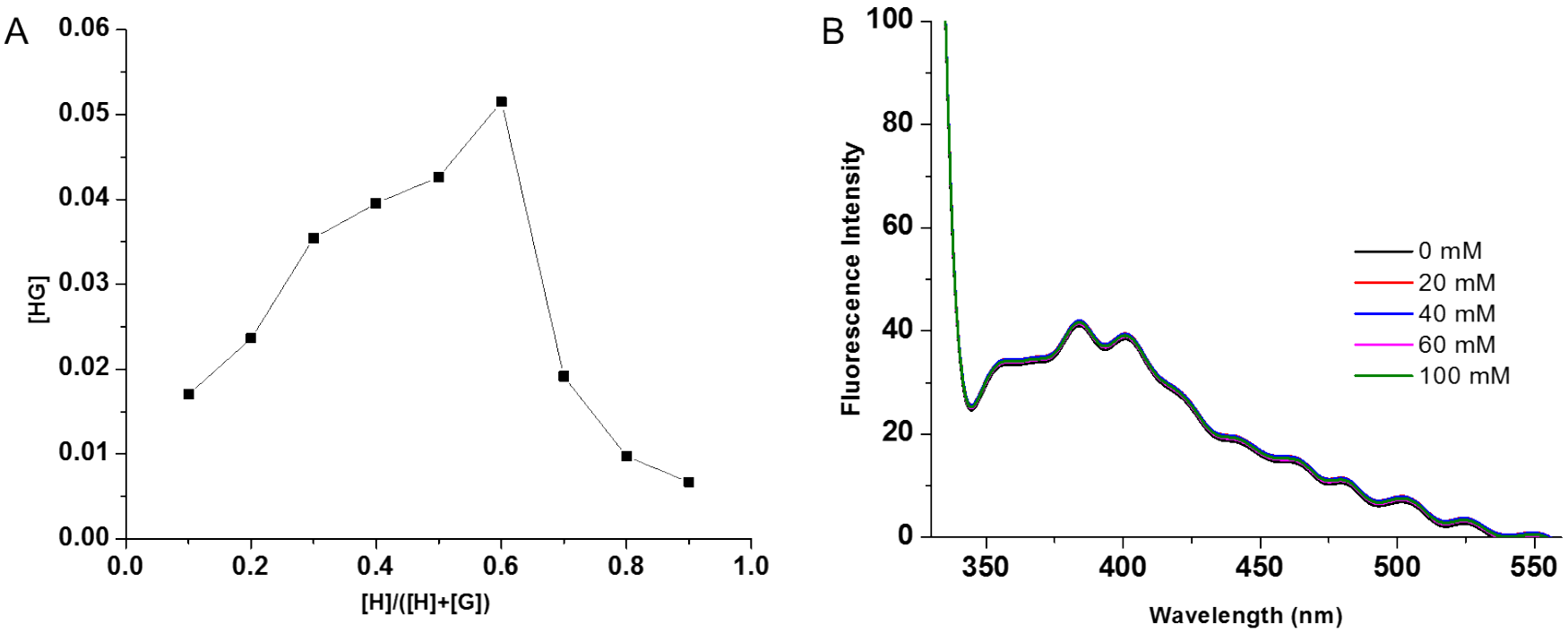


Figure S2: (A) Determination of stoichiometry of **2c**.spermine complex through job's plot. The maxima at 0.6 represent 2:1 stoichiometry; (B) Change in fluorescence intensity of **2c** in the presence of different amount of tetrabutylammonium perchlorate (0-100 mM).

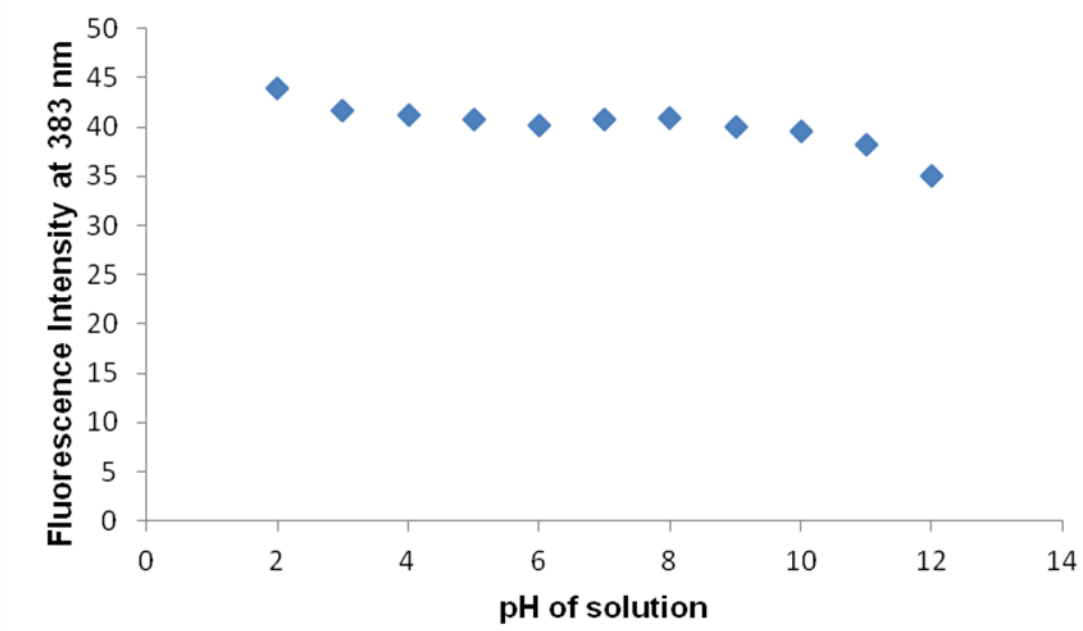


Figure S3: Effect of pH of the solution on emission profile of **2c**.

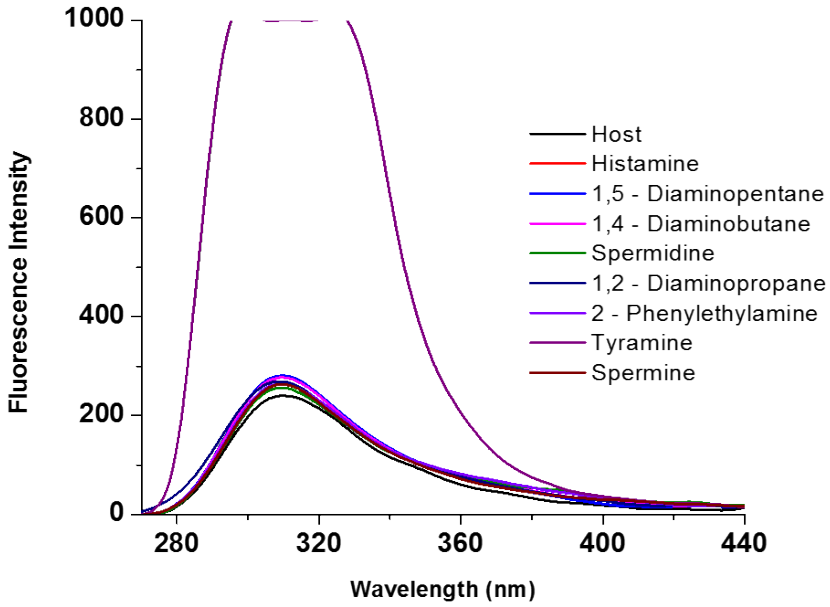


Figure S4: Change in fluorescence intensity of **2e** upon addition various biogenic amines (histamine, spermine, spermidine, tryamine, 1,2-Diaminopropane, 1,4-Diaminobutane, 1,5-Diaminopentane, 2-Phenylethylamine) in CH_3CN/H_2O (98:2; v/v) solvent system.

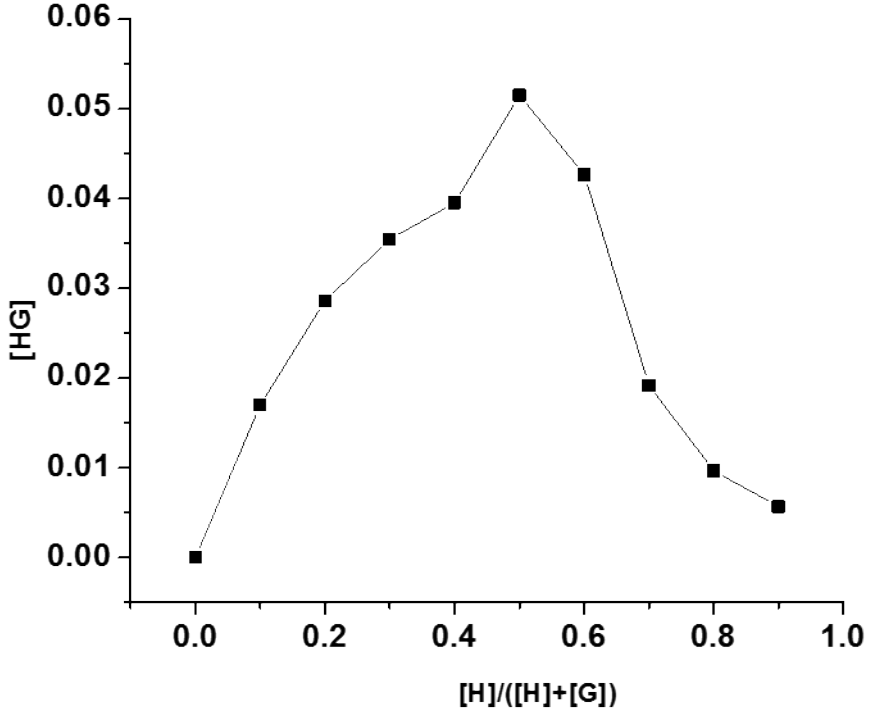


Figure S5: Determination of stoichiometry of **2d**.histamine complex through job's plot. The maxima at 0.5 represent 1:1 stoichiometry.

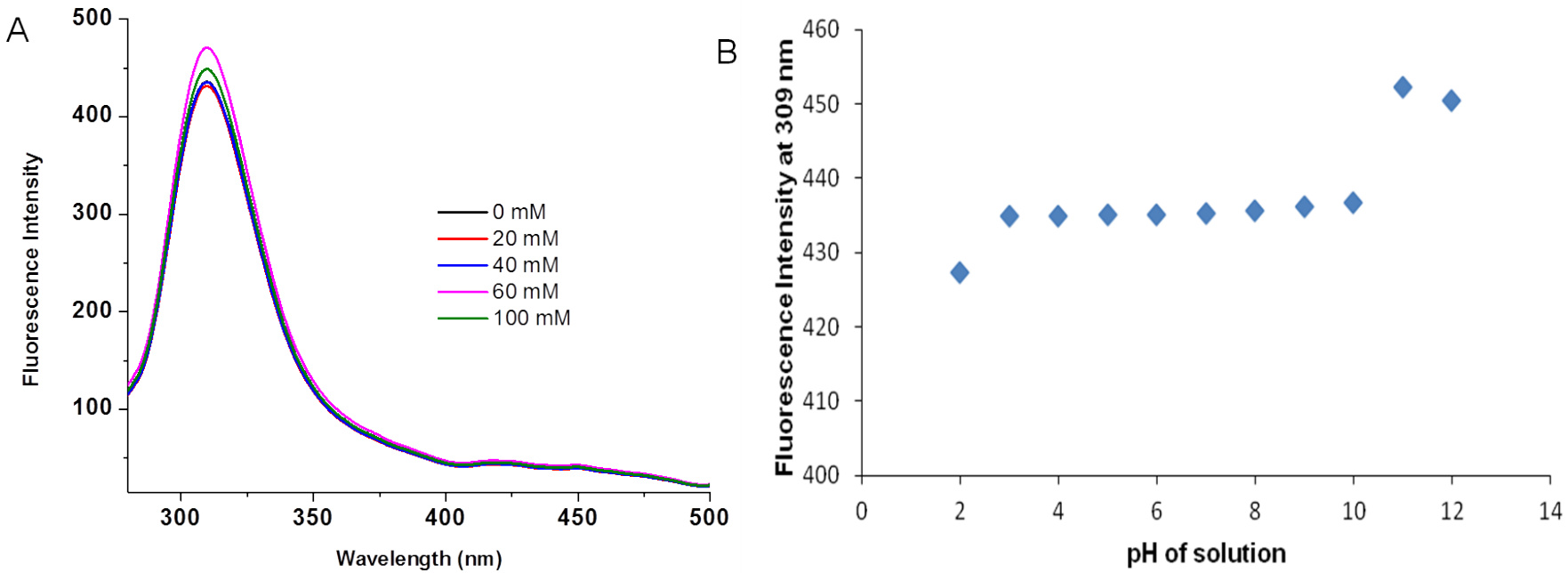


Figure S6: (A) Change in fluorescence intensity of **2d** in the presence of different amount of tetrabutylammonium perchlorate (0-100 mM); (B) Effect of pH of the solution on emission profile of **2d**.