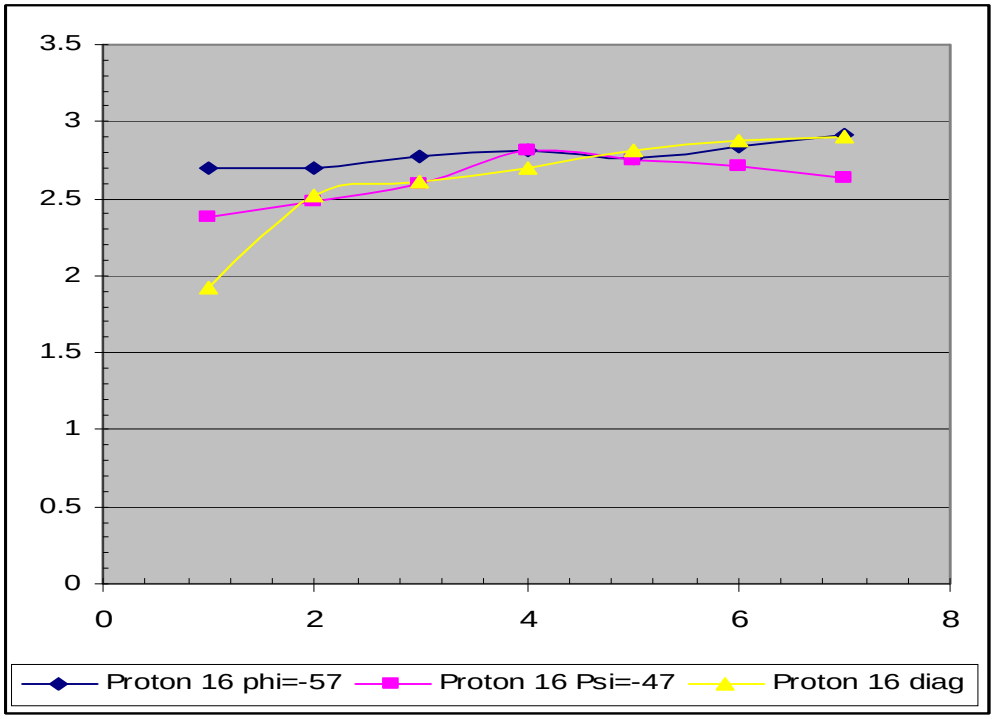
Phi -57	15	16	17	18	19
1	2.8165	2.7025	4.7646	4.2732	3.5145
2	2.9403	2.6976	4.4054	4.4471	3.6493
3	3.0279	2.7697	3.903	4.5903	3.8105
4	3.0104	2.8109	3.563	4.6102	4.0444
5	2.6997	2.7591	5.0645	4.1192	3.4006
6	2.6288	2.8404	5.2884	4.0231	3.2662
7	2.6206	2.9208	5.408	3.9743	3.1216

Psi -47	15	16	17	18	19
1	2.5429	2.3838	3.584	4.3108	3.46
2	2.5461	2.4834	4.0916	4.3372	3.49
3	2.655	2.5994	4.4567	4.3063	3.4967
4	3.0104	2.8109	3.563	4.6102	4.0444
5	3.0392	2.7474	5.0129	4.2501	3.5418
6	3.3458	2.7158	5.2123	4.2372	3.5723
7	3.6818	2.6291	5.3898	4.2335	3.6043

Diag	15	16	17	18	19
1	2.7586	1.9176	-0.4242	3.999	3.7119
2	2.8139	2.5206	2.7465	4.4879	3.7152
3	2.7706	2.6113	4.056	4.504	3.6292
4	2.8166	2.7026	4.7647	4.2732	3.5145
5	2.9088	2.8083	5.2805	4.1195	3.434
6	3.1201	2.8718	5.5681	4.0546	3.3375
7	3.4144	2.8982	5.6418	4.0213	3.2258

For the GLY-GLY as shown in Sheet-15, Phi and Psi angles are varied and the chemical shift values were calculated. When for each proton the Chemical shifts were plotted graphically, no clear trend emerged for systematizing the variations. Nor the numerical manipulation and averaging did yield any singular average structure in any simple way. Thus a need for knowing the functional dependence of the Chemical Shift with Phi-Psi angles became even more evident. For that matter if one tries to correlate the charge on the atom in a molecule with the chemical shift, no clear trends were immediately evident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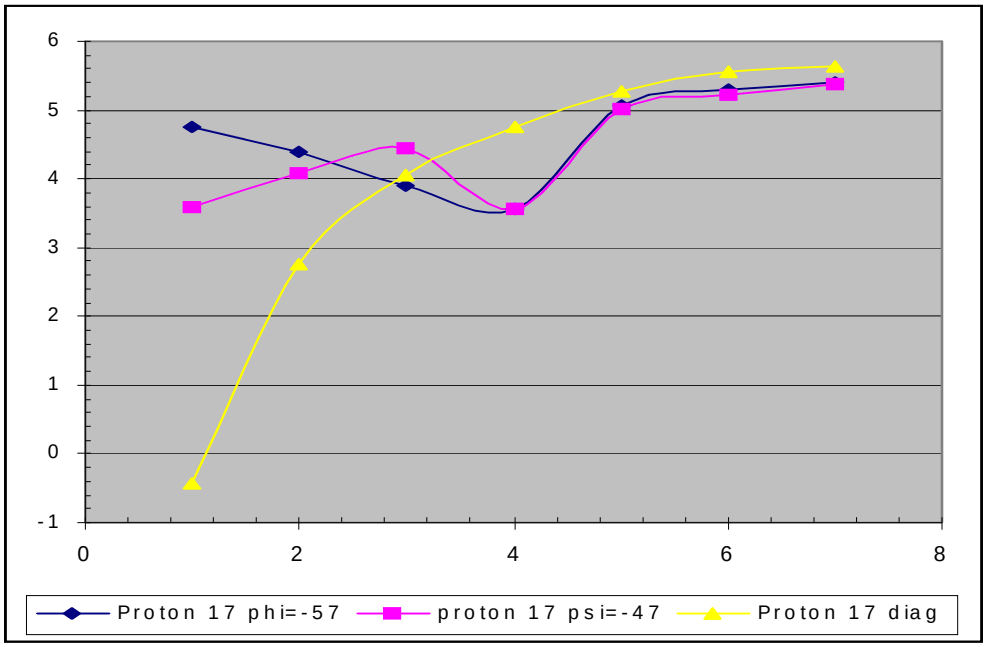
8
Proton 16 phi=-57
Proton 16 Psi=-47
Proton 16 diag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4
3
2
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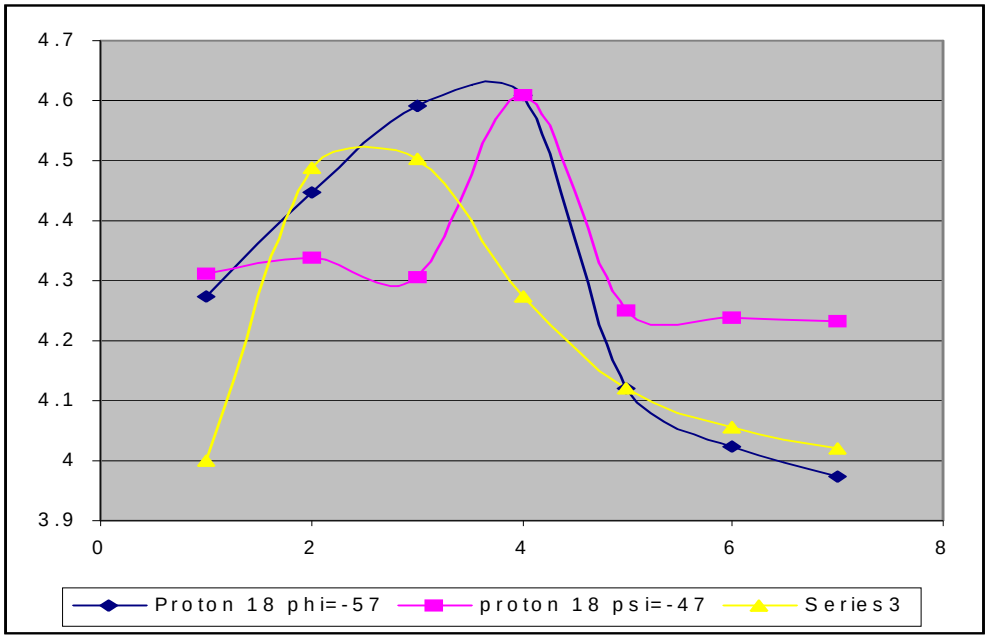
-1
0
2
4
6
8
Proton 17 phi=-57
proton 17 psi=-47
Proton 17 diag


4.7
4.6
4.5
4.4
4.3
4.2
4.1
4
3.9
0
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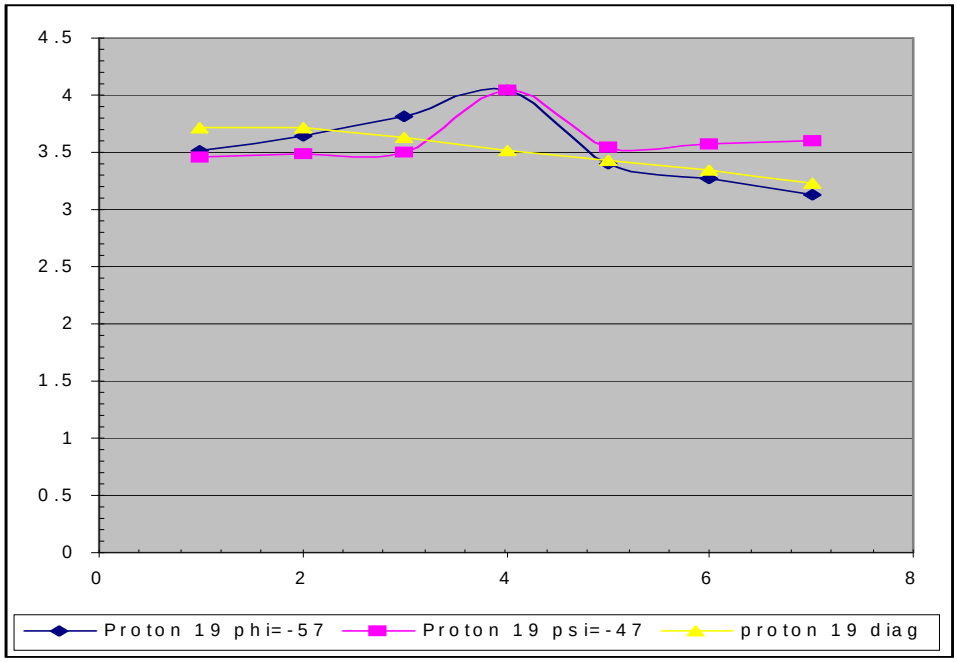
8
Proton 18 phi=-57
proton 18 psi=-47
Series3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4
3.5
3
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2
1.5
1
0.5
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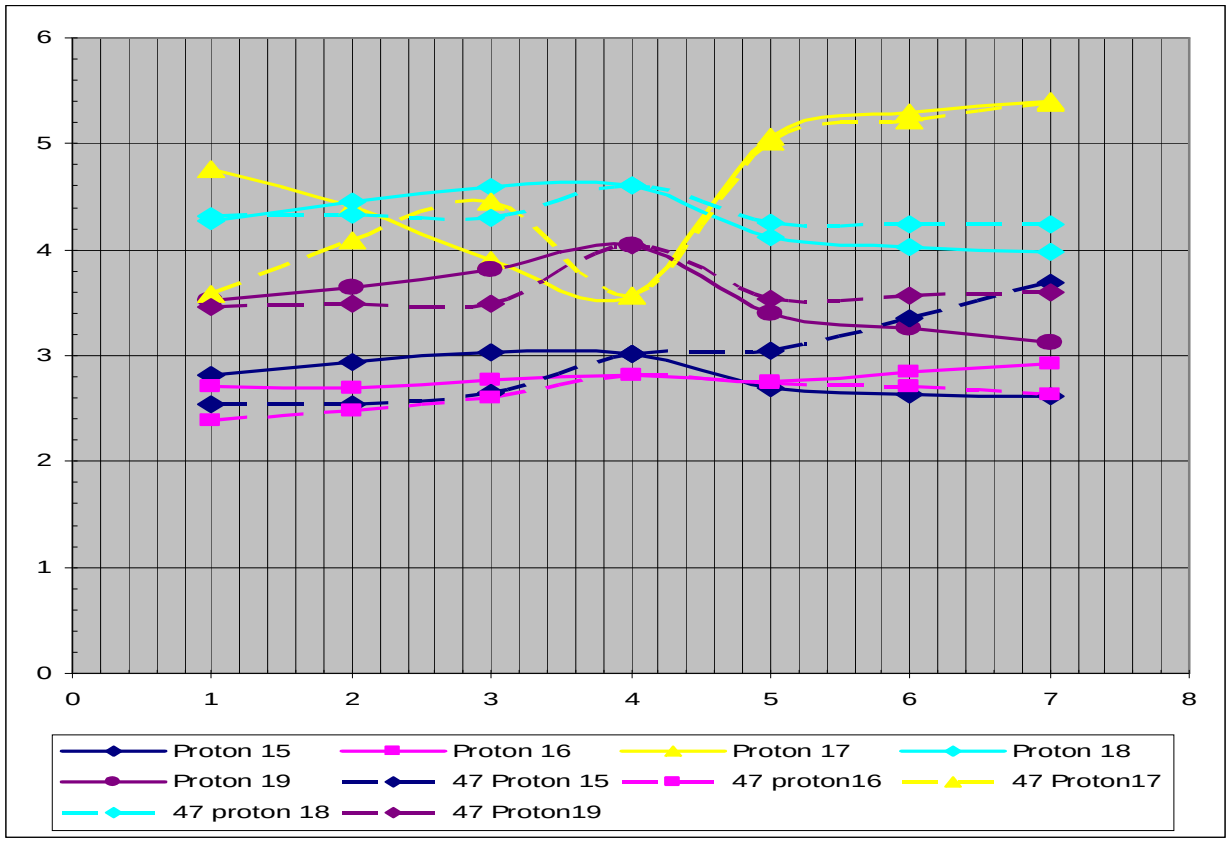
0
2
4
6
8
Proton 19 phi=-57
Proton 19 psi=-47
proton 19 diag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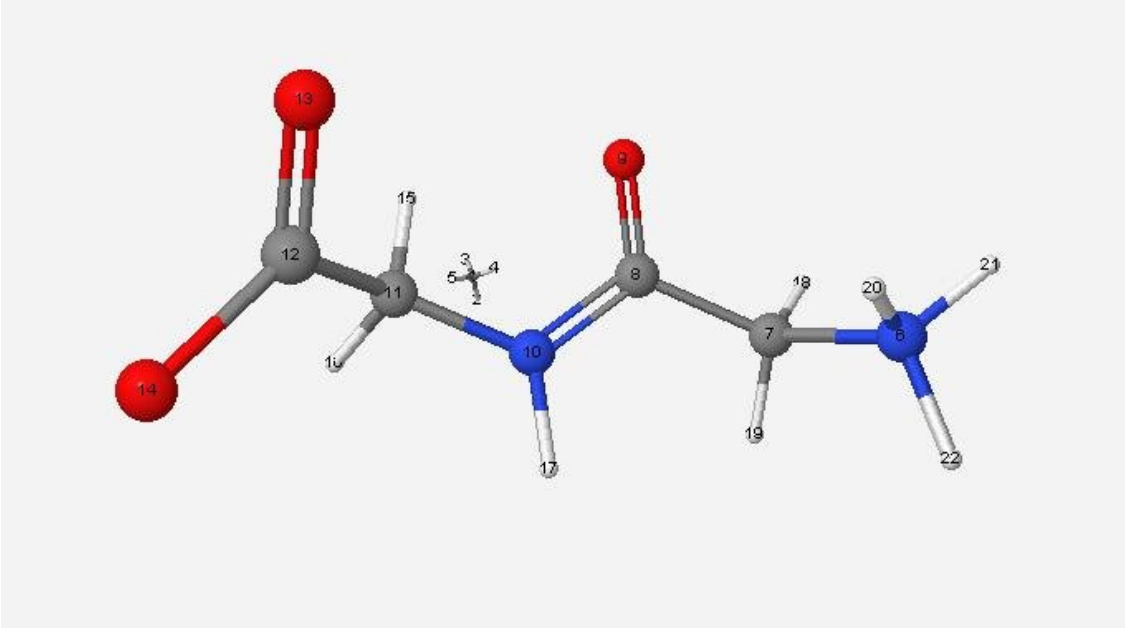
Proton 15
Proton 16
Proton 17
Proton 18
Proton 19
47 Proton 15
47 proton16
47 Proton17
47 proton 18
47 Proton19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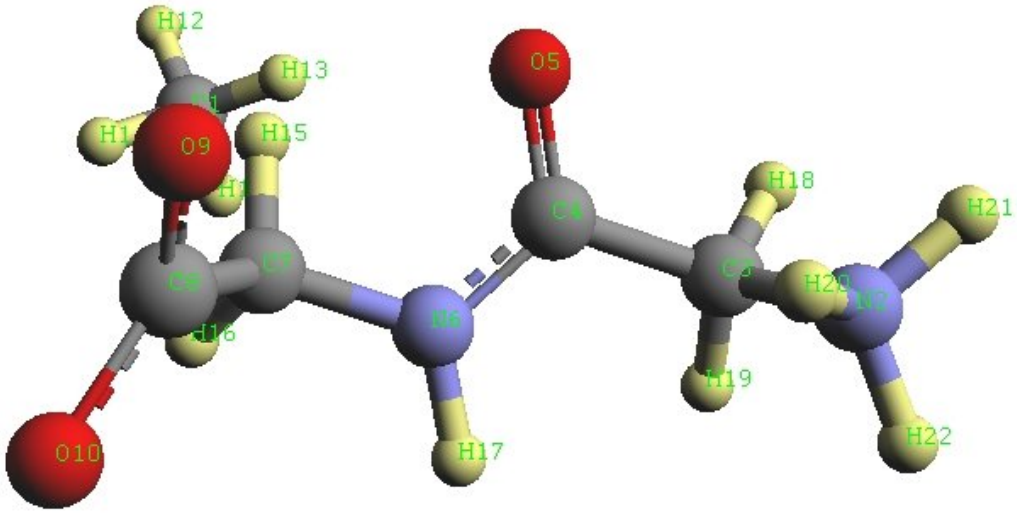
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H13
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H15
O9
H18
H21
C8
C7
C4
C2
H20
N6
H16
H19
O10
H17
H22