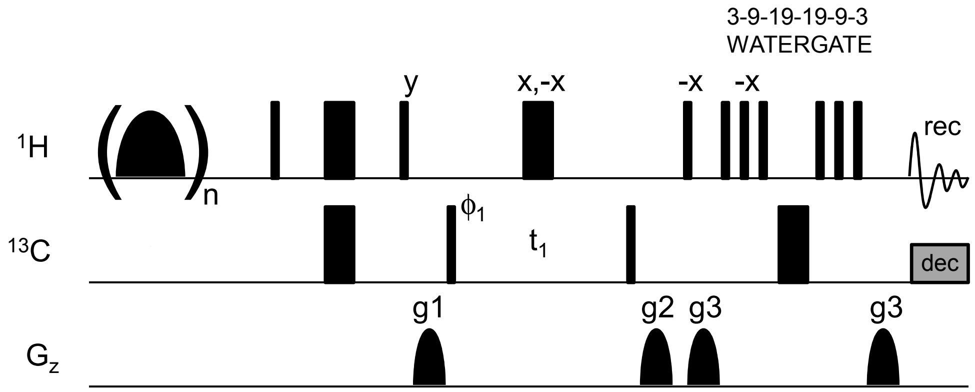
FIGURE S1

Pulse sequence for 2D STD-HSQC NMR



All phases are 'x' unless otherwise stated

ϕ_1 = x,-x (incremented for second dimension)

GARP ^{13}C decoupling was used during acquisition.

Water suppression was achieved using a 3-9-19-19-9-3 WATERGATE sequence directly before acquisition

Gradients g1 and g2 are purging gradients with a strength of 15 Gcm^{-1}
Gradient g3 is a WATERGATE selective gradient with a strength of 40 Gcm^{-1}

Receiver = x,-x,x,-x (control) or x,-x,-x,x (difference)

A comb of 'n' saturation pulses are applied over the required saturation period at the desired frequency offset to provide saturation transfer (on) or not (off).

Sat pulse = off,off,off,off (control)
= on,on,off,off (difference)

The pulse sequence above was used to create ^{13}C STD difference and control spectra using the hypercomplex (States) method for the indirect dimension.

FIGURE S2. 2D ^{13}C STD-HSQC NMR saturation transfer as a percentage of maximum transfer showing all positive values. Carbon resonances are listed as the edit point but all saturation transfers are through ^{1}H: this explains why single β, γ and δ carbons are shown twice for methylene based spin-systems containing two prochiral hydrogen atoms. Negative STD factors are shown with an asterisk (*)

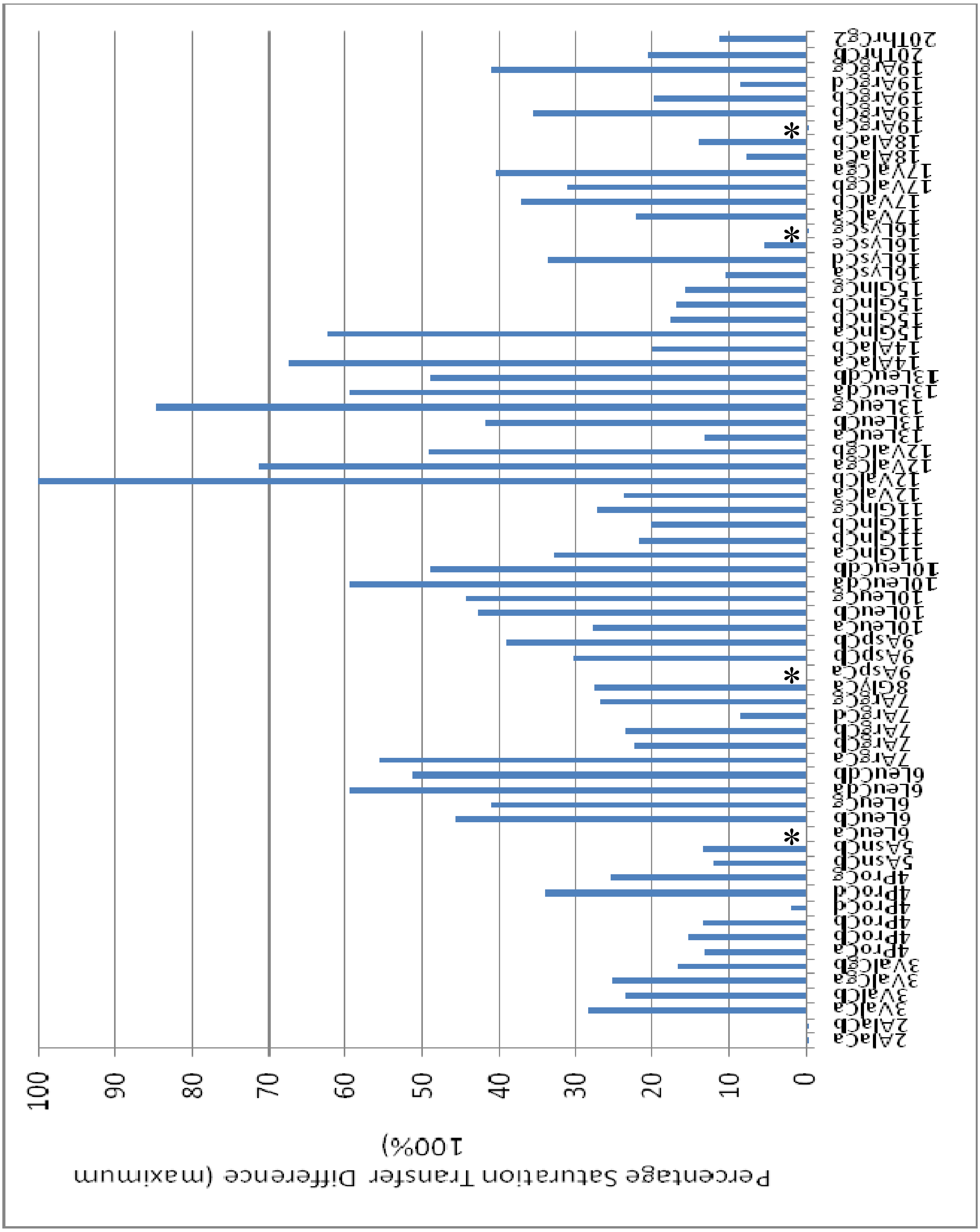


Table S1

NMR assignments of $^{15}N/^{13}C$-A20FMDV2 in 20 mM sodium dihydrogen-monohydrogen phosphate buffer at pH 6.5 containing 100 mM sodium chloride. ^{1}H referencing used the ^{1}H carrier centred on $^{1}H_2O$ (4.826 ppm from DSS at 10°C) and $^{13}C/^{15}N$ referencing completed using gyromagnetic gamma ratios (Wishart and Sykes, 1994, Methods in Enzymology 239, pg 363-392.)

Residue	N	H^N	H^α	Others
1Asn			4.712	$H^{\beta a/\beta b}$ 2.866, 2.930; C^β 37.506; $H^{\delta 2a/\delta 2b}$ 7.046, 7.766; $N^{\delta 2}$ 112.751
2Ala	118.516	8.719	4.404	C^α 51.388
3Val	121.860	8.373	4.403	C’ 176.451; C^α 62.460; H^β 2.105; C^β 31.634; $H^{\gamma a/\gamma b}$ 0.934, 1.055; $C^{\gamma a/\gamma b}$ 19.239, 20.190
4Pro				
5Asn	119.274	8.631	4.688	C’ 175.560; $H^{\beta a/\beta b}$ 2.813, 2.871; C^β 37.895; $H^{\delta 2a/\delta 2b}$ 7.000, 7.708; $N^{\delta 2}$ 112.940
6Leu	123.657	8.402	4.363	C’ 174.396; C^α 54.322; $H^{\beta a/\beta b}$ 1.696; C^β 41.311;H^γ 1.594; C^γ 25.713; $H^{\delta a/\delta b}$ 0.892, 0.935; $C^{\delta a/\delta b}$ 22.572, 24.085
7Arg	121.294	8.427	4.313	C’ 176.604; C^α 52.200; $H^{\beta a/\beta b}$ 1.807, 1.931; C^β 29.964; $H^{\gamma a/\gamma b}$ 1.654; C^γ 25.790; $H^{\delta a/\delta b}$ 3.240; C^δ 42.295; H^ε 7.471; N^ε 117.442
8Gly	109.896	8.429	3.957	C’ 176.158; C^α 44.716
9Asp	120.457	8.392	4.584	C’ 173.182; C^α 53.552; $H^{\beta a/\beta b}$ 2.754; C^β 39.976
10Leu	121.952	8.224	4.303	C’ 175.904; C^α 55.541; $H^{\beta a/\beta b}$ 1.706; C^β 41.303; H^γ 1.655; C^γ 26.054; $H^{\delta a/\delta b}$ 0.947, 0996; $C^{\delta a/\delta b}$ 22.257, 23.916
11Gln	121.142	8.374	4.289	C’ 176.461; C^α 55.071; $H^{\beta a/\beta b}$ 2.032, 2.101; C^β 28.222; $H^{\gamma a/\gamma b}$ 2.375; C^γ 32.936; $H^{\varepsilon 2a/\varepsilon 2b}$ 6.937, 7.651; $N^{\varepsilon 2}$ 112.990
12Val	121.838	8.146	4.024	C’ 175.458; C^α 62.189; H^β 2.088; C^β 31.828; $H^{\gamma a/\gamma b}$ 0.921, 1.014; $C^{\gamma a/\gamma b}$ 19.553, 20.5668
13Leu	125.407	8.299	4.340	C’ 175.770; C^α 54.228; $H^{\beta a/\beta b}$ 1.682; C^β 41.279;H^γ 1.600; C^γ 25.759; $H^{\delta a/\delta b}$ 0.895, 0.959; $C^{\delta a/\delta b}$ 22.401, 23.991

14Ala	124.435	8.256	4.282	C’ 176.474; C^{α} 51.920; H^{β} 1.407; C^{β} 18.381
15Gln	119.394	8.284	4.284	C’ 177.137; C^{α} 54.693; $H^{\beta a/\beta b}$ 1.997, 2.123; C^{β} 28.535; $H^{\gamma a/\gamma b}$ 2.416; C^{γ} 32.833; $H^{\varepsilon 2a/\varepsilon 2b}$ 6.958, 7.631; $N^{\varepsilon 2}$ 112.926
16Lys	123.025	8.379	4.289	C’ 175.310; C^{α} 55.156; $H^{\beta a/\beta b}$ 2.061, 2.365; C^{β} 26.397; $H^{\gamma a/\gamma b}$ 1.445; C^{γ} 23.877; $H^{\delta a/\delta b}$ 1.819; C^{δ} 31.972; $H^{\varepsilon a}$ 3.032; C^{ε} 41.159
17Val	121.959	8.221	4.091	C’ 175.666; C^{α} 61.405; H^{β} 2.084; C^{β} 17.969; $H^{\gamma a/\gamma b}$ 0.918, 0.989; $C^{\gamma a/\gamma b}$ 19.558, 20.246
18Ala	128.359	8.467	4.406	C’ 175.041; C^{α} 51.471
19Arg	121.233	8.462	4.401	C’ 176.735; C^{α} 58.847; $H^{\beta a/\beta b}$ 1.804, 1.919; C^{β} 29.617; $H^{\gamma a/\gamma b}$ 1.653; C^{γ} 25.306; $H^{\delta a/\delta b}$ 3.237; C^{δ} 42.605; H^{ε} 7.243; N^{ε} 117.559
20Thr	115.687	8.300	4.394	C’ 175.650; C^{α} 58.899; H^{β} 4.306; C^{β} 69.058; $H^{\gamma 1}$ 1.244; C^{γ} 20.678
21Hsl	118.587	8.745	4.735	C’ 173.467; C^{α} 69.209; $H^{\beta a/\beta b}$ 2.376, 2.646; C^{β} 29.328; $H^{\gamma a/\gamma b}$ 4.411, 4.588

Table S2

STD results [13]C-A20FMDV2. STD value = [(I – I_o) / I_o] x ligand excess where (I-I_o) = difference intensity, I_o = control intensity. Ligand excess = 400. I_o is multiplied by 16 to reflect the smaller number of transients used in the control. The ratio of control transients in difference and control experiments was 16:1. The number of transients were 256 and 8 for (I – I_o) and I_o respectively. All intensities were obtained using CCPN analysis.

Peak	Control	Difference	STD value
2AlaCa	316281	-31352	-2.4782
2AlaCb	-134981	88292	-16.3526
3ValCa	776160	42870	1.3808
3ValCb	5177500	237757	1.148
3ValCga	42003800	2052040	1.2214
3ValCgb	19243300	625718	0.813
4ProCa	1328290	33790	0.636
4ProCb	4215350	125012	0.7414
4ProCb	2161500	55855	0.646
4ProCd	2245400	7806	0.087
4ProCd	1451180	96076	1.6552
4ProCg	1842550	91262	1.2382
5AsnCb	3172870	74737	0.5888
5AsnCb	3286900	85334	0.649
6LeuCa			
6LeuCb	6802070	602830	2.2156
6LeuCda	53986800	6236600	2.888
6LeuCdb	45602600	4556980	2.4982
6LeuCg	7202190	573790	1.9918
7ArgCa	41962	4523	2.6944
7ArgCb	4521200	196720	1.0878
7ArgCb	4208640	192518	1.1436
7ArgCd	15986200	266753	0.4172
7ArgCg	7891830	410592	1.3006
8GlyCa	3459820	185121	1.3376
9AspCa	-59546	30270	-12.7088
9AspCb	2856910	167503	1.4658
9AspCb	3050290	231405	1.8966
10LeuCa	3538810	191088	1.35
10LeuCb	6912970	572909	2.0718
10LeuCda	53986800	6236600	2.888
10LeuCdb	50117500	4757340	2.373
10LeuCg	6480630	558172	2.1532
11GlnCa	3094470	196925	1.591

11GlnCb	4093150	172384	1.0528
11GlnCb	4388920	171934	0.9794
11GlnCg	3401340	179187	1.317
12ValCa	1736860	80067	1.1524
12ValCb	490099	95214	4.8568
12ValCga	7694740	1065130	3.4606
12ValCgb	27487000	2627450	2.3898
13LeuCa	2141020	54893	0.641
13LeuCb	4657200	376783	2.0226
13LeuCda	53986800	6236600	2.888
13LeuCdb	50117500	4757340	2.373
13LeuCg	1939950	319554	4.118
14AlaCa	943784	123810	3.2796
14AlaCb	17876400	692466	0.9684
15GlnCa	338105	41045	3.035
15GlnCb	3959620	136298	0.8606
15GlnCb	4225490	138633	0.8202
15GlnCg	7270210	221489	0.7616
16LysCa	1757720	35849	0.5098
16LysCd	2737570	179329	1.6376
16LysCe	8285240	89059	0.2688
16LysCg	1207010	-101044	-2.0928
17ValCa	1446650	62370	1.0778
17ValCb	235561	16919	1.7956
17ValCgb	40387800	2434690	1.507
17ValCga	41734700	3281750	1.9658
18AlaCa	1629250	24095	0.3698
18AlaCb	9950860	267546	0.6722
19ArgCa	940884	-19283	-0.5124
19ArgCb	2808800	192956	1.7174
19ArgCb	4148470	159292	0.96
19ArgCd	15986200	266753	0.4172
19ArgCg	7202190	573790	1.9918
20ThrCb	1309830	52450	1.001
20ThrCg2	19284100	426265	0.5526
21HslCa	149666	-9723	-1.624
21HslCg	590131	717723	3.0406
21HslCb	2210920	1457	0.0164
21HslCb	2762350	57547	0.5208

STD NMR data can be collected from the A20FMDV2-integrin αvβ6 interaction following previous observations (DiCara et al, 1997, J. Biol. Chem. **282**, 9657-9665 that confirmed an IC_{50} ~ 1 μM.). Identical conditions were used in this study.

Table S3

STD results ^{15}N-A20FMDV2. STD value = [(I – I_o) / I_o] x ligand excess where (I-I_o) = difference intensity, I_o = control intensity. Ligand excess = 400. I_o is multiplied by 16 to reflect the smaller number of transients used in the control. The ratio of control transients in difference and control experiments was 16:1. All intensities were obtained using CCPN analysis. ^{15}N-STD-HSQC spectra were run with 1024 data points (8000 Hz) in the direct F2 dimension and 64 pairs (1950 Hz) in the F1 dimension for 4 transients in the control experiments and 128 transients in the difference experiments.

Peak	Control	Difference	STD value
1AsnNH			
2AlaNH			
3ValNH	3776750	-1123000	-7.4336
4ProN			
5AsnNH	4117260	193000	1.1718
6LeuNH	3819950	151000	0.9882
7ArgNH	3796360	-656000	-4.32
8GlyNH	3320880	-155000	-1.1668
9AspNH	3786910	1469000	9.6978
10LeuNH	4349590	1455000	8.3628
11GlnNH	3189040	1638000	12.8408
12ValNH	3282830	1069000	8.1408
13LeuNH	2856180	1768900	15.483
14AlaNH	3479060	1335000	9.5932
15GlnNH	3361900	1757000	13.0656
16LysNH	3064720	1667000	13.5984
17ValNH	3483440	-426000	-3.0574
18AlaNH	3317220	1587000	11.9604
19ArgNH	3624360	1641000	11.3192
20ThrNH	3220020	813000	6.312
21HslNH	3517990	1127000	8.0088