

The example data presented here represents typical expected performance and is provided for the purposes of illustration and user guidance only. All Waters analytical instruments are installed and tested in accordance with Waters Standard Performance Tests. In presenting these data no agreement is implied by Waters to perform any additional non-standard performance tests during the installation.

XEVO TQ-XS: 6 Orders of Linear Dynamic Range

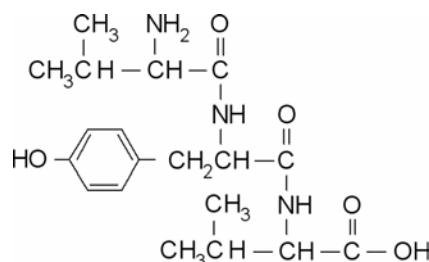
MRM Chromatographic Peak Area v Concentration

This document presents example data obtained using a Xevo TQ-XS with ACQUITY I-Class when performing an on column test in ESI positive MRM mode to demonstrate the linearity of response of the system configuration.

EXPERIMENTAL CONDITIONS

Sample: Val-Tyr-Val

$C_{19}H_{29}N_3O_5$



Dilution Series: 200ag/μl to 200pg/μl

Blank & Sample Diluent: H₂O + 0.01% Formic Acid

LC Conditions:

Instrument: ACQUITY I-Class
 Column: BEH C₁₈ 50mm x 150μm, 1.7μm
 Column Temperature: 40°C
 Injection volume: 5μL (Partial Loop-FTN)
 Mobile phase A: H₂O + 0.01% Formic Acid
 Mobile phase B: ACN + 0.01 % Formic Acid
 Wash: ACN + 0.01 % Formic Acid
 Purge: H₂O + 0.01% Formic Acid
 Seal Wash: H₂O: ACN 90:10
 Flow rate: 800μL/min

Gradient:

Time (min)	%A	%B	Curve
0.00	90	10	-
0.20	90	10	6
1.20	75	25	6
1.21	90	10	6
1.70	90	10	6
15.0	90	10	6

MS Conditions

Instrument: Xevo TQ-XS
Ionisation mode: ESI positive
Source Temperature: 150°C
Desolvation Temperature: 650°C
Cone Gas Flow : 150L/Hr
Desolvation Gas Flow: 1000L/Hr
Resolution: MS1 and MS2 0.70 +/- 0.10Da (FWHM)
Detector Gain : 0.1
MS Acquisition: MRM transition m/z 380.25 > 136.00, 200ms dwell, 1.7min
Cone Voltage: 20V
Collision Energy: 25eV

Software MassLynx 4.2 SCN943

RESULTS

The lower limit of quantitation (LLOQ) was determined as 200ag/μl (1fg on-column) based on the lowest concentration producing S: N >10:1 (RMS) and peak area > 5x blank.

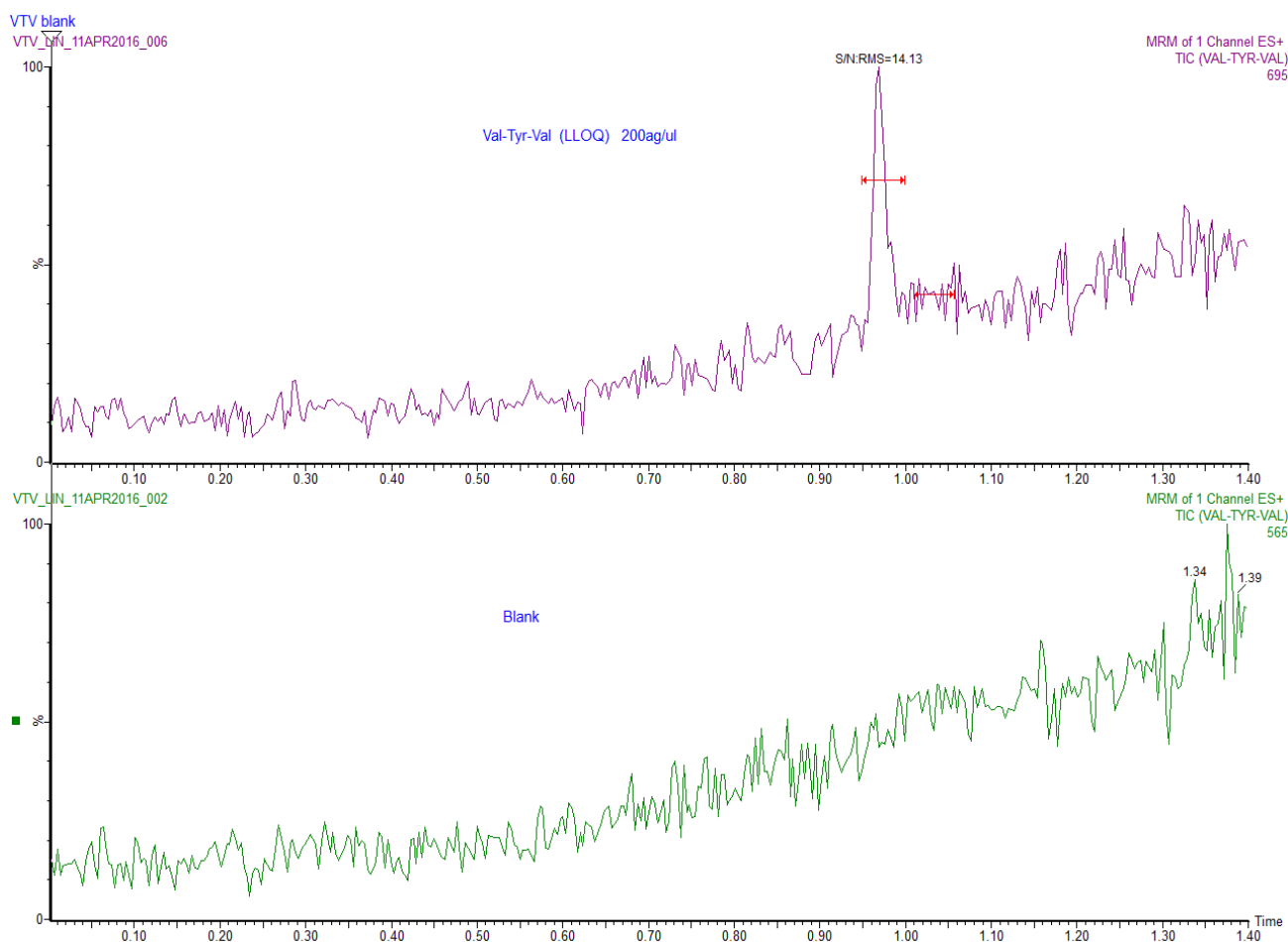


Figure1. Example chromatogram for LLOQ (200ag/μl) S: N >10:1 (RMS) and peak area > 5x Blank.

Data was acquired for triplicate injections of the blank and each of the 19 sample dilutions points covering a 6 order range from 200ag/μl to 200pg/μl.

TargetLynx XS was used to process the data:

The plot below shows the MRM chromatographic peak area to be linear v sample concentration over 6 orders with a correlation co-efficient (r^2) = 0.998 and back-calculated deviation of <15% for all 57 data points from the $1/x^2$ weighted line of fit.

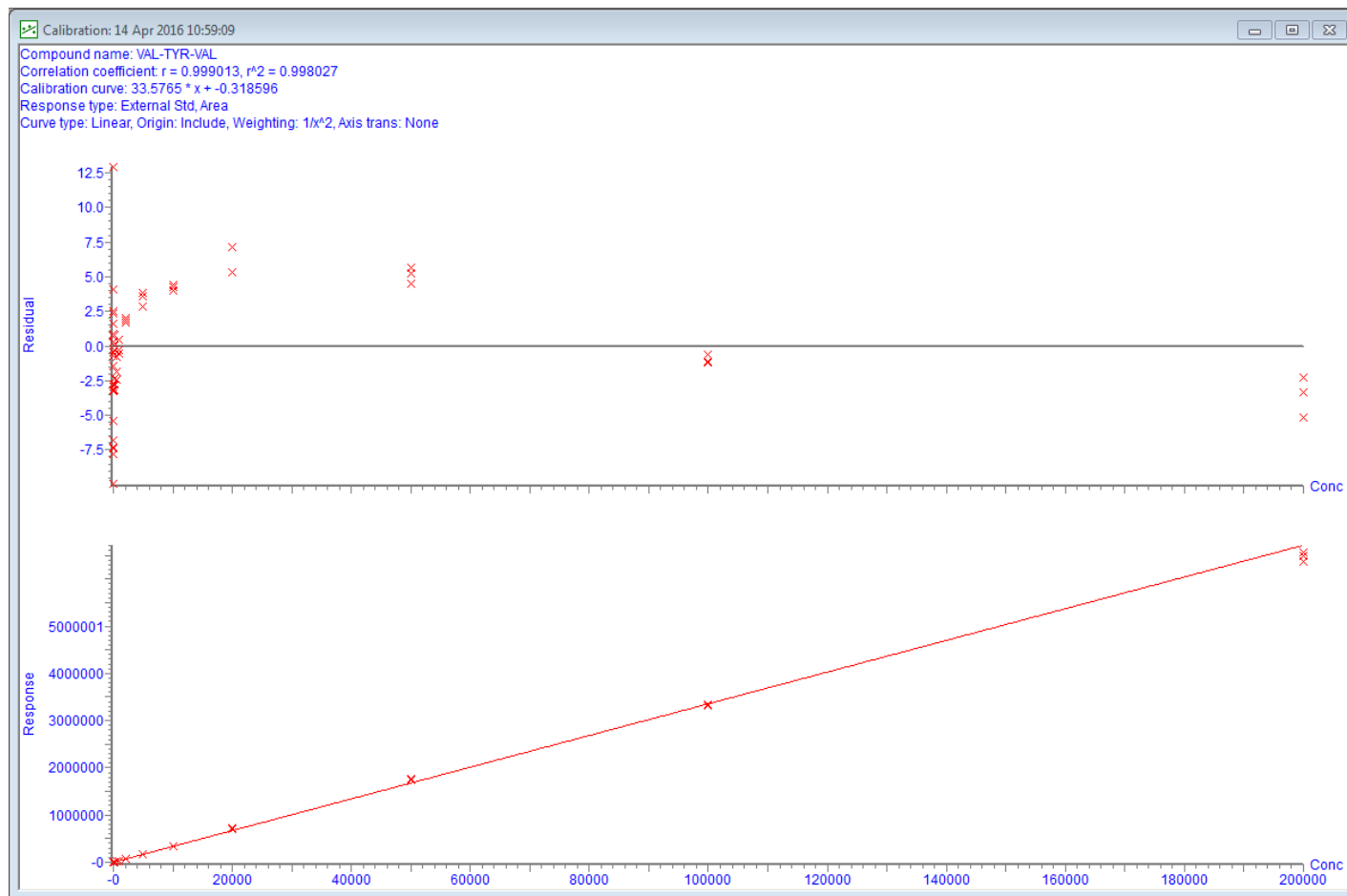


Figure2. TargetLynx XS plot of MRM chromatographic peak area v Val-Tyr-Val sample concentration.

The TargetLynx XS statistical data for the individual injections is shown below. No detectable blank response was observed and no data points required exclusion or manual integration.

	#	Name	Type	Std. Conc	RT	Height	Area	Primary Flags	Conc.	%Dev
1	1	VTV_LIN_11APR2016_001	Blank							
2	2	VTV_LIN_11APR2016_002	Blank							
3	3	VTV_LIN_11APR2016_003	Blank							
4	4	VTV_LIN_11APR2016_004	Standard	0.200	0.97	291	6	bb	0.185	-7.3
5	5	VTV_LIN_11APR2016_005	Standard	0.200	0.97	258	6	bb	0.180	-9.9
6	6	VTV_LIN_11APR2016_006	Standard	0.200	0.97	342	7	bb	0.226	12.9
7	7	VTV_LIN_11APR2016_007	Standard	0.500	0.97	768	17	bb	0.513	2.5
8	8	VTV_LIN_11APR2016_008	Standard	0.500	0.97	793	17	bb	0.504	0.8
9	9	VTV_LIN_11APR2016_009	Standard	0.500	0.97	757	16	bb	0.473	-5.4
10	10	VTV_LIN_11APR2016_010	Standard	1.000	0.97	1559	33	bb	1.003	0.3
11	11	VTV_LIN_11APR2016_011	Standard	1.000	0.97	1572	34	bb	1.024	2.4
12	12	VTV_LIN_11APR2016_012	Standard	1.000	0.97	1592	34	bb	1.016	1.6
13	13	VTV_LIN_11APR2016_013	Standard	2.000	0.97	3118	66	bb	1.985	-0.7
14	14	VTV_LIN_11APR2016_014	Standard	2.000	0.97	3193	70	bb	2.082	4.1
15	15	VTV_LIN_11APR2016_015	Standard	2.000	0.97	3066	65	bb	1.941	-3.0
16	16	VTV_LIN_11APR2016_016	Standard	5.000	0.97	7943	165	bb	4.928	-1.4
17	17	VTV_LIN_11APR2016_017	Standard	5.000	0.97	7738	166	bb	4.965	-0.7
18	18	VTV_LIN_11APR2016_018	Standard	5.000	0.97	7834	169	bd	5.042	0.8
19	19	VTV_LIN_11APR2016_019	Standard	12.500	0.97	18261	391	bb	11.644	-6.8
20	20	VTV_LIN_11APR2016_020	Standard	12.500	0.97	17982	388	bb	11.579	-7.4
21	21	VTV_LIN_11APR2016_021	Standard	12.500	0.97	18126	387	bb	11.523	-7.8
22	22	VTV_LIN_11APR2016_022	Standard	20.000	0.97	30156	650	bb	19.366	-3.2
23	23	VTV_LIN_11APR2016_023	Standard	20.000	0.97	30354	649	bb	19.341	-3.3
24	24	VTV_LIN_11APR2016_024	Standard	20.000	0.97	31434	676	bb	20.141	0.7
25	25	VTV_LIN_11APR2016_025	Standard	50.000	0.97	75791	1632	bb	48.617	-2.8
26	26	VTV_LIN_11APR2016_026	Standard	50.000	0.97	77014	1632	bb	48.626	-2.7
27	27	VTV_LIN_11APR2016_027	Standard	50.000	0.97	78651	1671	bb	49.768	-0.5
28	28	VTV_LIN_11APR2016_028	Standard	100.000	0.97	153967	3266	bb	97.276	-2.7
29	29	VTV_LIN_11APR2016_029	Standard	100.000	0.97	158648	3358	bb	100.028	0.0
30	30	VTV_LIN_11APR2016_030	Standard	100.000	0.97	153131	3249	bb	96.784	-3.2
31	31	VTV_LIN_11APR2016_031	Standard	200.000	0.97	319806	6766	bb	201.513	0.8
32	32	VTV_LIN_11APR2016_032	Standard	200.000	0.97	308626	6559	bb	195.341	-2.3
33	33	VTV_LIN_11APR2016_033	Standard	200.000	0.97	317652	6693	bb	199.343	-0.3
34	34	VTV_LIN_11APR2016_034	Standard	500.000	0.97	790179	16661	bb	496.220	-0.8
35	35	VTV_LIN_11APR2016_035	Standard	500.000	0.97	778052	16377	bb	487.757	-2.4
36	36	VTV_LIN_11APR2016_036	Standard	500.000	0.97	779274	16483	bb	490.905	-1.8
37	37	VTV_LIN_11APR2016_037	Standard	1000.000	0.97	1582039	33385	bb	994.300	-0.6
38	38	VTV_LIN_11APR2016_038	Standard	1000.000	0.97	1589329	33490	bb	997.441	-0.3
39	39	VTV_LIN_11APR2016_039	Standard	1000.000	0.97	1599140	33741	bb	1004.901	0.5
40	40	VTV_LIN_11APR2016_040	Standard	2000.000	0.97	3254890	68522	bb	2040.790	2.0
41	41	VTV_LIN_11APR2016_041	Standard	2000.000	0.97	3251331	68287	bb	2033.793	1.7
42	42	VTV_LIN_11APR2016_042	Standard	2000.000	0.97	3234445	68421	bb	2037.779	1.9
43	43	VTV_LIN_11APR2016_043	Standard	5000.000	0.97	8275694	172716	bb	5143.957	2.9
44	44	VTV_LIN_11APR2016_044	Standard	5000.000	0.97	8266890	173956	bb	5180.902	3.6
45	45	VTV_LIN_11APR2016_045	Standard	5000.000	0.97	8331474	174356	bb	5192.796	3.9
46	46	VTV_LIN_11APR2016_046	Standard	10000.000	0.97	16635004	349110	bb	10397.460	4.0
47	47	VTV_LIN_11APR2016_047	Standard	10000.000	0.97	16743059	350541	bb	10440.064	4.4
48	48	VTV_LIN_11APR2016_048	Standard	10000.000	0.97	16595026	350088	bb	10426.585	4.3
49	49	VTV_LIN_11APR2016_049	Standard	20000.000	0.96	34093340	719718	bb	21435.174	7.2
50	50	VTV_LIN_11APR2016_050	Standard	20000.000	0.96	33304974	707504	bb	21071.406	5.4
51	51	VTV_LIN_11APR2016_051	Standard	20000.000	0.97	34027476	719204	bb	21419.847	7.1
52	52	VTV_LIN_11APR2016_052	Standard	50000.000	0.96	82482288	1767449	bb	52639.423	5.3
53	53	VTV_LIN_11APR2016_053	Standard	50000.000	0.96	82950088	1754829	bb	52263.572	4.5
54	54	VTV_LIN_11APR2016_054	Standard	50000.000	0.97	83303096	1774078	bb	52836.852	5.7
55	55	VTV_LIN_11APR2016_055	Standard	100000.000	0.96	154207504	3316584	bb	98776.890	-1.2
56	56	VTV_LIN_11APR2016_056	Standard	100000.000	0.96	155068720	3335634	bb	99344.250	-0.7
57	57	VTV_LIN_11APR2016_057	Standard	100000.000	0.96	153526688	3321434	bb	98921.321	-1.1
58	58	VTV_LIN_11APR2016_058	Standard	200000.000	0.96	293406464	6565345	bb	195533.787	-2.2
59	59	VTV_LIN_11APR2016_059	Standard	200000.000	0.96	286716992	6367684	bb	189646.921	-5.2
60	60	VTV_LIN_11APR2016_060	Standard	200000.000	0.96	291799296	6488689	bb	193250.763	-3.4

Figure3. TargetLynx XS exported statistical data for dilution series Val-Tyr-Val 200ag/μl to 200pg/μl

The same data is shown below after reprocessing (Excel) as a Log-Log plot in order to allow the line of fit to be more easily visualized over the 6 order range.

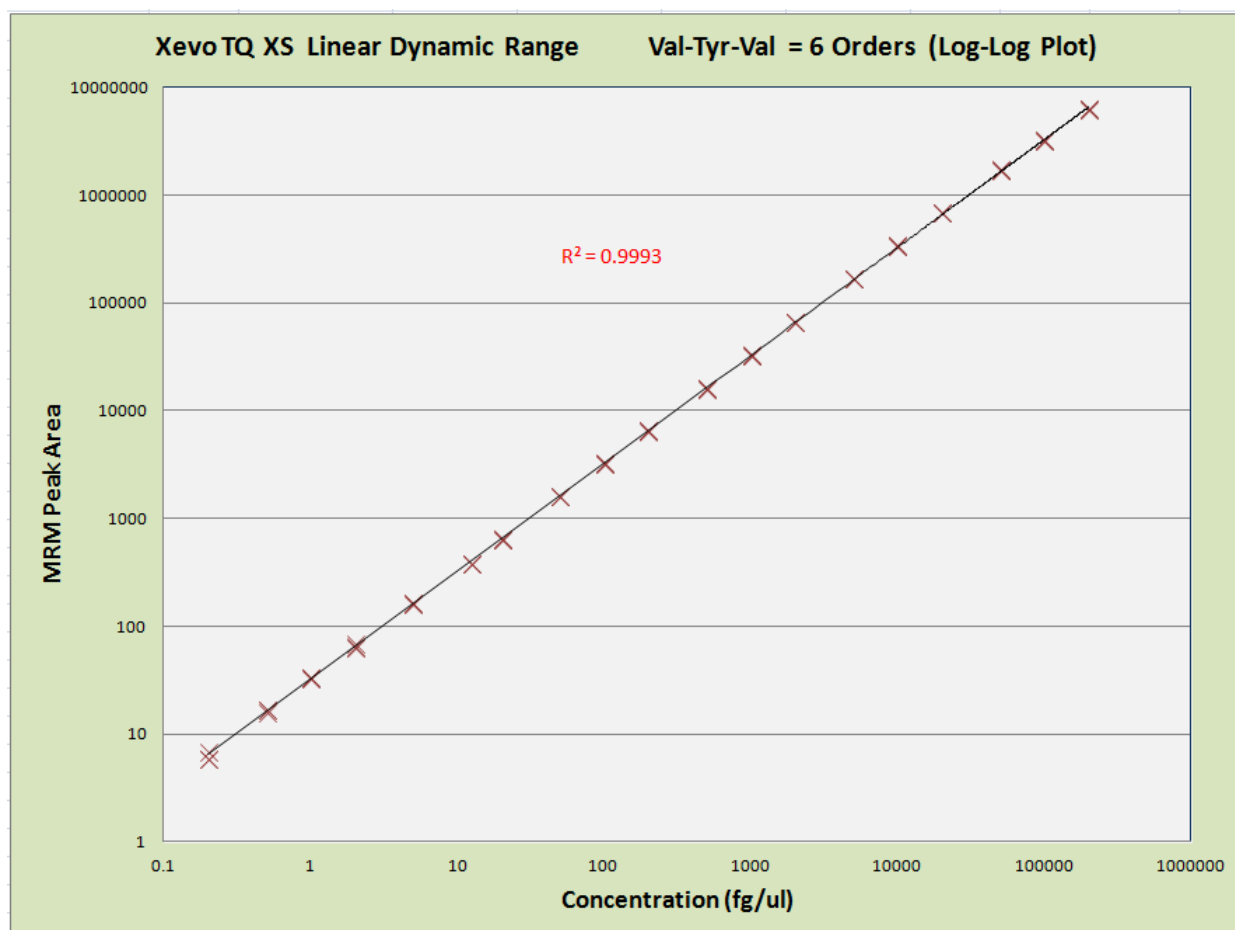


Figure 4. Peak area v sample concentration Val-Tyr-Val 200ag/μl to 200pg/μl shown as Log-Log plot



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