	SVM_R of the OSC transformed data PREDICTIONS	Samples ID	Samples Brand Name	Mean of 10 Spectra/capsule	Total Pill Mass	Actual PREDICTED Doxycycline content in the Pill
0	277.0184629	16k_0000250	caredoxy			
1	277.0196538	16k_0000250	caredoxy			
2	277.0197072	16k_0000250	caredoxy			
3	277.0183973	16k_0000250	caredoxy			
4	277.0184004	16k_0000250	caredoxy			
5	277.0185544	16k_0000250	caredoxy			
6	277.0183855	16k_0000250	caredoxy			
7	277.0184326	16k_0000250	caredoxy			
8	277.0183954	16k_0000250	caredoxy			
9	277.0184775	16k_0000250	caredoxy	**277**	700	**0.39571429**
10	277.0183797	16k_0000251	caredoxy			
11	277.0183818	16k_0000251	caredoxy			
12	277.0183797	16k_0000251	caredoxy			
13	277.0183797	16k_0000251	caredoxy			
14	277.0183799	16k_0000251	caredoxy			
15	277.0183898	16k_0000251	caredoxy			
16	277.0183827	16k_0000251	caredoxy			
17	277.0183835	16k_0000251	caredoxy			
18	277.0183802	16k_0000251	caredoxy			
19	277.0183822	16k_0000251	caredoxy	**277**	700	**0.39571429**
20	277.0183797	16k_0000253	caredoxy			

21	277.0183799	16k_0000253	caredoxy			
22	277.0183813	16k_0000253	caredoxy			
23	277.0183836	16k_0000253	caredoxy			
24	277.0183838	16k_0000253	caredoxy			
25	277.0183954	16k_0000253	caredoxy			
26	277.0183814	16k_0000253	caredoxy			
27	277.0183835	16k_0000253	caredoxy			
28	277.0183798	16k_0000253	caredoxy			
29	277.0183849	16k_0000253	caredoxy			
30	277.0183809	16k_0000253	caredoxy	277	700	0.39571429
31	277.0311092	16k_0000259	caredoxy			
32	277.0377734	16k_0000259	caredoxy			
33	277.0284808	16k_0000259	caredoxy			
34	277.0669999	16k_0000259	caredoxy			
35	277.0201155	16k_0000259	caredoxy			
36	277.0247876	16k_0000259	caredoxy			
37	277.0322173	16k_0000259	caredoxy			
38	277.0259134	16k_0000259	caredoxy			
39	277.029446	16k_0000259	caredoxy	277	700	0.39571429
40	277.0184103	16k_0000264	caredoxy			
41	277.01842	16k_0000264	caredoxy			
42	277.0183842	16k_0000264	caredoxy			
43	277.0183868	16k_0000264	caredoxy			
44	277.0184914	16k_0000264	caredoxy			
45	277.0183808	16k_0000264	caredoxy			
46	277.0188213	16k_0000264	caredoxy			
47	277.0184348	16k_0000264	caredoxy			
48	277.0185292	16k_0000264	caredoxy			
49	277.0183995	16k_0000264	caredoxy	277	700	0.39571429
50	464.8938763	19k_0000133	caredoxy			
51	437.0762472	19k_0000133	caredoxy			
52	438.6728295	19k_0000133	caredoxy			

53	430.9793169	19k_0000133	caredoxy			
54	419.0059424	19k_0000133	caredoxy			
55	363.6164705	19k_0000133	caredoxy			
56	347.8605856	19k_0000133	caredoxy			
57	383.4448585	19k_0000133	caredoxy			
58	381.2507199	19k_0000133	caredoxy			
59	463.4087278	19k_0000133	caredoxy	413	700	0.59
60	426.8090763	19k_0000135	caredoxy			
61	315.7258227	19k_0000135	caredoxy			
62	330.263851	19k_0000135	caredoxy			
63	374.2375728	19k_0000135	caredoxy			
64	316.930781	19k_0000135	caredoxy			
65	346.7096702	19k_0000135	caredoxy			
66	354.9802247	19k_0000135	caredoxy			
67	312.2213885	19k_0000135	caredoxy			
68	395.0517664	19k_0000135	caredoxy			
69	413.7451205	19k_0000135	caredoxy			
70	425.1639625	19k_0000135	caredoxy			
71	426.5154443	19k_0000135	caredoxy	369	700	0.52714286
72	387.3296796	19k_0000139cg	Doxyzim			
73	391.3848181	19k_0000139cg	Doxyzim			
74	391.8014686	19k_0000139cg	Doxyzim			
75	388.3684211	19k_0000139cg	Doxyzim			
76	385.2888829	19k_0000139cg	Doxyzim			
77	382.674364	19k_0000139cg	Doxyzim			
78	393.3940858	19k_0000139cg	Doxyzim			
79	375.0043669	19k_0000139cg	Doxyzim			
80	388.9737139	19k_0000139cg	Doxyzim			
81	397.1969496	19k_0000139cg	Doxyzim	388	700	0.55428571
82	441.5489144	19k_0000139bw	Doxyzim			
83	433.6457898	19k_0000139bw	Doxyzim			
84	417.0664108	19k_0000139bw	Doxyzim			
85	428.2417853	19k_0000139bw	Doxyzim			

86	429.412063	19k_0000139bw	Doxyzim			
87	434.8817199	19k_0000139bw	Doxyzim			
88	437.1017648	19k_0000139bw	Doxyzim			
89	437.6515766	19k_0000139bw	Doxyzim			
90	429.2003873	19k_0000139bw	Doxyzim			
91	431.4221381	19k_0000139bw	Doxyzim	**432**	700	**0.61714286**
92	446.4102469	19k_0000147	Doxycyclin			
93	399.1239124	19k_0000147	Doxycyclin			
94	423.1399166	19k_0000147	Doxycyclin			
95	416.0386014	19k_0000147	Doxycyclin			
96	410.8066177	19k_0000147	Doxycyclin			
97	412.9888684	19k_0000147	Doxycyclin			
98	430.1095909	19k_0000147	Doxycyclin			
99	419.112564	19k_0000147	Doxycyclin			
100	441.1426443	19k_0000147	Doxycyclin			
101	422.6883663	19k_0000147	Doxycyclin			
102	430.3035749	19k_0000147	Doxycyclin			
103	438.7633445	19k_0000147	Doxycyclin	**424**	700	**0.60571429**
104	371.1551726	21L-0001	DoxyNext			
105	286.8099676	21L-0001	DoxyNext			
106	345.2137384	21L-0001	DoxyNext			
107	332.5442658	21L-0001	DoxyNext			
108	317.7375069	21L-0001	DoxyNext			
109	355.329908	21L-0001	DoxyNext			
110	288.3965685	21L-0001	DoxyNext			
111	300.2730158	21L-0001	DoxyNext			
112	347.4336441	21L-0001	DoxyNext			
113	299.8197867	21L-0001	DoxyNext	**324**	700	**0.46285714**
114	292.1984021	21L-0008	DoxyNext			
115	292.1194257	21L-0008	DoxyNext			
116	359.1156957	21L-0008	DoxyNext			
117	311.3031221	21L-0008	DoxyNext			
118	309.5428321	21L-0008	DoxyNext			

119	288.4736966	21L-0008	DoxyNext			
120	327.6537768	21L-0008	DoxyNext			
121	317.394051	21L-0008	DoxyNext			
122	341.3829017	21L-0008	DoxyNext			
123	300.4157695	21L-0008	DoxyNext	**313**	700	**0.44714286**
124	300.9257402	19K-0576	EDOXY			
125	299.8674496	19K-0576	EDOXY			
126	298.5298451	19K-0576	EDOXY			
127	287.6182172	19K-0576	EDOXY			
128	299.4977517	19K-0576	EDOXY			
129	300.7957049	19K-0576	EDOXY			
130	300.9760578	19K-0576	EDOXY			
131	298.2397775	19K-0576	EDOXY			
132	300.5303071	19K-0576	EDOXY			
133	297.1977766	19K-0576	EDOXY	**298**	700	**0.42571429**
134	288.3863054	19K-0570	DOXYCYCLI			
135	284.6924135	19K-0570	DOXYCYCLI			
136	278.3588073	19K-0570	DOXYCYCLI			
137	289.8133237	19K-0570	DOXYCYCLI			
138	281.671617	19K-0570	DOXYCYCLI			
139	281.0243062	19K-0570	DOXYCYCLI			
140	280.7279912	19K-0570	DOXYCYCLI			
141	277.4894909	19K-0570	DOXYCYCLI			
142	277.7955734	19K-0570	DOXYCYCLI			
143	282.0561129	19K-0570	DOXYCYCLI	**282**	700	**0.40285714**
144	452.9240972	19K-0551	caredoxy			
145	403.2648527	19K-0551	caredoxy			
146	428.4781896	19K-0551	caredoxy			
147	440.3185212	19K-0551	caredoxy			
148	427.9120509	19K-0551	caredoxy			
149	430.576697	19K-0551	caredoxy			
150	400.7610855	19K-0551	caredoxy			
151	356.2020185	19K-0551	caredoxy			

152	445.2939884	19K-0551	caredoxy			
153	339.1044545	19K-0551	caredoxy	**412**	700	**0.58857143**
154	293.3566869	17m-0055	N/A			
155	295.8294372	17m-0055	N/A			
156	293.4752182	17m-0055	N/A			
157	296.1284746	17m-0055	N/A			
158	280.8495289	17m-0055	N/A			
159	296.0051153	17m-0055	N/A			
160	292.9849813	17m-0055	N/A			
161	293.4760013	17m-0055	N/A			
162	308.9230633	17m-0055	N/A			
163	311.593482	17m-0055	N/A	**296**	700	**0.42285714**
164	391.989414	17m-0049	N/A			
165	287.2001088	17m-0049	N/A			
166	357.4210478	17m-0049	N/A			
167	417.6331158	17m-0049	N/A			
168	392.4858869	17m-0049	N/A			
169	422.6654841	17m-0049	N/A			
170	385.1208108	17m-0049	N/A			
171	390.6986363	17m-0049	N/A			
172	411.4528145	17m-0049	N/A			
173	389.6158587	17m-0049	N/A	**384**	700	**0.54857143**
174	449.5532433	17m-0047	N/A			
175	300.6018272	17m-0047	N/A			
176	390.5499366	17m-0047	N/A			
177	326.679902	17m-0047	N/A			
178	322.7473747	17m-0047	N/A			
179	360.4256011	17m-0047	N/A			
180	464.5420438	17m-0047	N/A			
181	391.2541691	17m-0047	N/A			
182	342.1272806	17m-0047	N/A			
183	407.6783723	17m-0047	N/A	**375**	700	**0.53571429**
184	474.8558321	16-1075	microdox			

185	279.1986537	16-1075	microdox			
186	352.9562531	16-1075	microdox			
187	435.5506633	16-1075	microdox			
188	469.3267643	16-1075	microdox			
189	333.4523161	16-1075	microdox			
190	371.842946	16-1075	microdox			
191	352.3716267	16-1075	microdox			
192	345.0714355	16-1075	microdox			
193	456.352034	16-1075	microdox			
194	293.0053037	16-1075	microdox	378	700	0.54
195	277.018913	16-1073	caredoxy			
196	277.0190969	16-1073	caredoxy			
197	277.02005	16-1073	caredoxy			
198	277.0207094	16-1073	caredoxy			
199	277.0189634	16-1073	caredoxy			
200	277.0191087	16-1073	caredoxy			
201	277.0208994	16-1073	caredoxy			
202	277.0305584	16-1073	caredoxy			
203	277.0290401	16-1073	caredoxy			
204	277.0197211	16-1073	caredoxy	277	700	0.39571429
205	363.700768	16-0789	microdox			
206	399.1612924	16-0789	microdox			
207	399.9488315	16-0789	microdox			
208	443.3391942	16-0789	microdox			
209	388.5450379	16-0789	microdox			
210	363.0982807	16-0789	microdox			
211	394.1833276	16-0789	microdox			
212	464.7952227	16-0789	microdox			
213	363.2087258	16-0789	microdox			
214	337.6008507	16-0789	microdox	391	700	0.55857143
215	468.685727	16-0787	asdoxin			
216	371.9486406	16-0787	asdoxin			
217	392.9617947	16-0787	asdoxin			

218	432.954922	16-0787	asdoxin			
219	460.1963996	16-0787	asdoxin			
220	461.6820539	16-0787	asdoxin			
221	282.1212773	16-0787	asdoxin			
222	435.5065998	16-0787	asdoxin			
223	438.421178	16-0787	asdoxin			
224	473.14991	16-0787	asdoxin	**421**	700	**0.60142857**
225	386.7121758	16-0786	microdox			
226	329.0312962	16-0786	microdox			
227	484.7390925	16-0786	microdox			
228	419.3915943	16-0786	microdox			
229	374.1188677	16-0786	microdox			
230	388.9046521	16-0786	microdox			
231	387.341378	16-0786	microdox			
232	421.2184309	16-0786	microdox			
233	394.8145391	16-0786	microdox			
234	394.1570996	16-0786	microdox	398	700	**0.56857143**
235	277.0184259	16-0777	caredoxy			
236	277.0197677	16-0777	caredoxy			
237	277.0206549	16-0777	caredoxy			
238	277.0184244	16-0777	caredoxy			
239	277.0188549	16-0777	caredoxy			
240	277.018535	16-0777	caredoxy			
241	277.0191609	16-0777	caredoxy			
242	277.0186053	16-0777	caredoxy			
243	277.0189494	16-0777	caredoxy			
244	277.0198735	16-0777	caredoxy	**277**	700	**0.39571429**
245	341.5920219	16-0776	doxycycline			
246	327.7447251	16-0776	doxycycline			
247	345.3275496	16-0776	doxycycline			
248	314.3579998	16-0776	doxycycline			
249	315.2808039	16-0776	doxycycline			
250	291.9650996	16-0776	doxycycline			

251	287.7330428	16-0776	doxycycline			
252	309.0642477	16-0776	doxycycline			
253	299.7643697	16-0776	doxycycline			
254	348.5831603	16-0776	doxycycline			
255	277.0185147	16-0776	doxycycline	314	700	**0.44857143**
256	277.0183839	16-0680	N/A			
257	277.0183804	16-0680	N/A			
258	277.0183798	16-0680	N/A			
259	277.0184005	16-0680	N/A			
260	277.0183798	16-0680	N/A			
261	277.0183821	16-0680	N/A			
262	277.0183799	16-0680	N/A			
263	277.0183797	16-0680	N/A			
264	277.0184043	16-0680	N/A			
265	277.0183797	16-0680	N/A	**277**	700	**0.39571429**
266	277.0183797	16-0656	N/A			
267	277.0183802	16-0656	N/A			
268	277.0183818	16-0656	N/A			
269	277.0183798	16-0656	N/A			
270	277.0183798	16-0656	N/A			
271	277.0183808	16-0656	N/A			
272	277.0183798	16-0656	N/A			
273	277.0183797	16-0656	N/A			
274	277.0183809	16-0656	N/A			
275	277.0183799	16-0656	N/A	**277**	700	**0.39571429**
276	308.0825976	16-0619	alldox			
277	291.9810734	16-0619	alldox			
278	291.4499942	16-0619	alldox			
279	291.7964274	16-0619	alldox			
280	292.0591964	16-0619	alldox			
281	303.0164162	16-0619	alldox			
282	291.0759068	16-0619	alldox			
283	296.1586916	16-0619	alldox			

284	292.9517628	16-0619	alldox			
285	293.169615	16-0619	alldox			
286	291.2328961	16-0619	alldox	294	700	**0.42**
287	284.3539277	16-0252	N/A			
288	380.3331179	16-0252	N/A			
289	284.4494592	16-0252	N/A			
290	325.0732948	16-0252	N/A			
291	293.3450594	16-0252	N/A			
292	296.8473684	16-0252	N/A			
293	344.1149911	16-0252	N/A			
294	377.0589682	16-0252	N/A			
295	410.3493955	16-0252	N/A			
296	295.9488795	16-0252	N/A	329	700	**0.47**

Models Development Data Summary

Actual doxycycline content	Total Pill Mass	Actual Doxycycline content in the Pill
100	700	0.142857143
200	700	0.285714286
300	700	0.428571429
500	700	0.714285714

Sample ID	Doxycycline Total Pill Mass (mg)	Doxycycline Dosage form (mg)	Expected Doxycycline content in the Pill	Lowest Mass Doxycycline API	Lower Limit	Highest Mass Doxycycline API	Upper Limit
21L-0005	309.43	100	0.32317487	90	0.290857383	120	0.38780984
21L-0009	258.99	100	0.38611529	90	0.347503765	120	0.46333835
21L-0004	322.18	100	0.3103855	90	0.279346949	120	0.3724626
21L-0007	293.37	100	0.34086648	90	0.306779834	120	0.40903978
21L-0010	230.41	100	0.43400894	90	0.390608047	120	0.52081073
21L-0012	274.28	100	0.36459093	90	0.328131836	120	0.43750911
21L-0001	292.89	100	0.34142511	90	0.307282598	120	0.40971013
21L-0003	289.15	100	0.34584126	90	0.311257133	120	0.41500951
21L-0008	195.71	100	0.51096009	90	0.459864085	120	0.61315211
21L-0011	311.04	100	0.32150206	90	0.289351852	120	0.38580247
21L-0013	294.71	100	0.33931662	90	0.305384955	120	0.40717994

21L-0002	304.57	100	0.32833175	90	0.295498572	120	0.3939981
21L-0006	322.18	100	0.3103855	90	0.279346949	120	0.3724626

Total mass   **3698.91**

Mean   **284.531538**

Api Content   **0.35145489**

Api Content

RANGE	0.27934695	0.613152113