

Photochemical reaction mechanisms of 2-nitrobenzyl compounds: 2-Nitrobenzyl alcohols form 2-nitroso hydrates by dual proton transfer

Martin Gaplovsky, Yuri V. Il'ichev,* Svetlana V. Kombarova, Marek Mac, Markus A. Schwörer and Jakob Wirz*

Supplementary Information

Table S1. Total Energies (hartree) in the Gas Phase, Total Free Energies in Water, Scaled Zero-Point Energies (sZPE), and Energies and Imaginary Frequencies ($i\omega$) for Transition Structures for Isomers of 2-Nitrobenzyl alcohol (**1**, R = H) and 1-(2-Nitrophenyl)ethanol (**1**, R = Me).

Molecule	B3LYP/6-31G(d)// B3LYP/6-31G(d)	sZPE kJ mol ⁻¹	$i\omega$ cm ⁻¹	B3LYP/6-311+G(2d,p)// B3LYP/6-31G(d)	PCM (Water) ^a B3LYP/6-311+G(2d,p)// B3LYP/6-31G(d)
R = H					
<i>anti</i> - 1	-551.268180	357.9		-551.450238	-551.468192
<i>syn</i> - 1	-551.270682	360.3		-551.451676	-551.465262
<i>E,E</i> - 2	-551.229525	354.0		-551.419587	-551.439691
<i>E,Z</i> - 2'	-551.216452	352.7		-551.406471	-551.428901
<i>E,Z</i> - 2	-551.241320	352.3		-551.428620	-551.440095
<i>Z,E</i> - 2	-551.222581	354.1		-551.411790	-551.430659
<i>Z,Z</i> - 2'	-551.213408	352.9		-551.403660	-551.424646
<i>Z,Z</i> - 2	-551.227867	355.1		-551.415031	-551.427424
<i>syn</i> - 3	-551.254751	353.7		-551.439136	-551.456805
<i>anti</i> - 3	-551.251898	353.1		-551.436930	-551.458270
<i>cis</i> - 5'	-551.256950	357.1		-551.442996	-551.474464
<i>cis</i> - 5	-551.260945	357.8		-551.445438	-551.470408
<i>trans</i> - 5'	-551.254923	357.1		-551.441425	-551.472843
<i>trans</i> - 5	-551.257427	357.2		-551.443061	-551.471175
6'	-551.281360	356.4		-551.466593	-551.478068
6	-551.284512	356.5		-551.470037	-551.493896
TS[<i>E,E</i> - 2 - <i>cis</i> - 5']	-551.209311	352.6	242.8	-551.398398	-551.424879
TS[<i>E,Z</i> - 2' - <i>trans</i> - 5']	-551.193345	348.8	361.2	-551.382945	-551.410317
TS[<i>E,Z</i> - 2 - <i>trans</i> - 5]	-551.205075	347.1	336.9	-551.392133	-551.411703
TS[<i>E,Z</i> - 2 - <i>syn</i> - 3]	-551.240338	342.7	768.4	-551.427738	-551.440601
TS[<i>cis</i> - 5 - <i>trans</i> - 5]	-551.228050	355.9	441.8	-551.414439	-551.438010
R = Me					
<i>anti</i> - 1	-590.584965	432.2		-590.777158	-590.792447
<i>syn</i> - 1	-590.586276	433.9		-590.778426	-590.789811
<i>E,E</i> - 2	-590.539948	425.8		-590.740519	-590.760582
<i>E,Z</i> - 2'	-590.536265	424.7		-590.736887	-590.753172

<i>E,Z</i> - 2	-590.559971	423.3	-590.758804	-590.771031
<i>syn</i> - 3	-590.571696	427.6	-590.768358	-590.783314
<i>cis</i> - 5'	-590.577666	428.8	-590.774269	-590.800212
<i>trans</i> - 5'	-590.576445	428.7	-590.772861	-590.789440
<i>trans</i> - 5	-590.579683	429.2	-590.775781	-590.794964
TS [<i>E,E</i> - 2 - <i>cis</i> - 5']	-590.525784	424.8	195.3 -590.725668	-590.749268
TS [<i>E,Z</i> - 2 - <i>trans</i> - 5]	-590.528749	422.9	220.9 -590.727318	-590.741309

Anions (R = H)	B3LYP/6-31+G(d)// sZPE / B3LYP/6-31+G(d) kJ mol ⁻¹	<i>i</i> ω / cm ⁻¹	B3LYP/6-311+G(2d,p)// B3LYP/6-31+G(d)	PCM (Water) ^a B3LYP/6-311+G(2d,p)// B3LYP/6-31+G(d)
<i>E</i> - 2 ⁻	-550.727062	317.6	-550.881103	-550.979025
<i>cis</i> - 5 ⁻	-550.743365	314.1	-550.894682	-551.010204
TS [<i>E</i> - 2 ⁻ - <i>cis</i> - 5 ⁻]	-550.681152	314.8	423.0 -550.833633	-550.943172
<i>Z</i> - 2 ⁻	-550.741956	317.3	-550.896412	-550.983543
<i>trans</i> - 5 ⁻	-550.744218	314.7	-550.895307	-551.007651
TS [<i>Z</i> - 2 ⁻ - <i>trans</i> - 5 ⁻]	-550.682088	312.8	620.2 -550.834421	-550.939744
<i>syn</i> - 3 ⁻	-550.744856	317.2	-550.899370	-550.984699
<i>anti</i> - 3 ⁻	-550.739009	314.4	-550.892206	-550.976414
TS [<i>Z</i> - 2 ⁻ - <i>syn</i> - 3 ⁻]	-550.740726	307.8	956.2 -550.896026	-550.983393
6' ⁻	-550.741080	316.9	-550.891805	-550.996498
6 ⁻	-550.744883	315.4	-550.895773	-551.000044
OH ⁻	-75.796681	21.9	-75.827741	-75.988680
H ₂ O	-76.422572	55.4	-76.459460	-76.469888

^a Total free energy (gas-phase plus solvation free energy) at 298 K.

Table S2. The B3LYP/6-31G(d) harmonic vibrational frequencies scaled with a factor of 0.9613 and relative intensities for **1** (R=H) and its isomers.

anti-1		syn-1		E,E-2		E,Z-2'		E,Z-2		Z,Z-2'		Z,Z-2		syn-3		anti-3				
No.	ν/cm^{-1}	rel.int.	ν/cm^{-1}	rel.int.	ν/cm^{-1}	rel.int.	ν/cm^{-1}	rel.int.	ν/cm^{-1}	rel.int.	ν/cm^{-1}	rel.int.	ν/cm^{-1}	rel.int.	ν/cm^{-1}	rel.int.	ν/cm^{-1}	rel.int.		
1	23	1.5	52	0.8	86	1.2	98	1.5	88	1.0	57	0.0	87	0.1	82	1.9	88	0.6	61	2.9
2	115	0.0	111	1.1	102	3.8	106	0.3	109	4.1	110	2.4	101	2.2	114	2.9	119	2.1	98	4.9
3	172	1.9	141	3.2	174	1.4	164	0.4	170	1.1	167	0.0	164	0.3	171	0.8	159	8.5	122	1.1
4	214	100.7	197	4.3	218	2.2	190	50.1	238	75.9	229	1.9	214	28.0	237	2.9	240	6.8	189	1.3
5	222	7.6	251	4.1	251	1.2	237	5.2	254	32.2	249	37.9	227	8.1	282	1.0	257	2.3	257	4.3
6	237	41.5	299	0.6	274	4.0	257	56.4	283	2.4	255	2.0	248	55.1	311	11.7	282	9.4	270	7.0
7	279	1.8	339	1.1	292	166.9	310	42.7	318	13.4	351	24.3	305	35.6	352	9.5	333	5.2	340	0.4
8	368	0.3	394	0.1	369	21.2	331	94.6	359	6.4	352	13.3	332	58.3	392	7.4	359	52.6	378	8.9
9	389	2.9	427	1.5	372	92.0	350	29.9	373	2.1	362	133.2	359	55.7	409	56.1	398	109.0	394	28.3
10	425	0.0	496	2.0	388	4.0	414	3.9	445	8.3	409	65.0	412	7.0	451	10.9	441	1.5	431	58.3
11	476	1.9	510	53.5	392	0.5	469	4.2	475	3.4	411	1.1	450	14.0	479	13.1	479	9.4	455	8.3
12	537	0.6	547	80.7	472	0.1	473	2.3	491	2.5	468	5.3	499	0.8	493	7.2	489	3.9	470	68.4
13	583	9.7	588	22.1	515	5.6	507	14.7	516	2.6	518	12.4	518	7.9	503	6.5	528	114.7	529	7.7
14	664	13.1	652	5.7	528	2.1	538	7.3	575	2.4	524	14.1	531	6.3	555	1.6	558	118.6	584	75.8
15	666	0.3	687	18.5	569	4.0	567	2.7	613	4.4	570	7.3	575	14.5	610	2.7	583	14.0	584	49.7
16	713	50.8	731	31.6	601	18.1	597	20.7	684	1.2	600	14.4	596	20.5	649	17.8	648	23.3	637	11.8
17	767	2.6	775	11.0	681	5.2	678	7.9	692	6.8	682	3.2	674	2.6	671	3.8	703	23.3	716	20.0
18	777	12.2	789	10.6	717	23.1	693	4.4	721	48.0	714	12.7	684	4.3	706	124.3	722	8.0	730	14.8
19	836	25.3	840	25.2	734	45.3	711	38.3	794	3.1	738	42.9	713	28.8	721	13.8	752	49.1	761	45.3
20	863	0.2	868	0.8	802	14.0	778	7.6	831	13.8	803	7.9	784	4.8	794	4.2	831	37.7	813	32.8
21	942	2.1	930	21.8	803	0.5	810	23.0	886	3.8	808	0.1	811	21.1	840	18.9	859	4.0	865	2.5
22	968	0.2	940	20.4	810	7.8	820	40.9	922	0.5	817	3.2	844	14.1	886	45.7	919	2.4	898	67.9
23	1003	0.0	964	0.4	929	0.3	916	34.2	946	7.6	933	0.4	919	2.8	902	100.7	953	26.6	936	3.1
24	1026	31.3	1035	1.7	937	231.2	926	164.4	960	174.3	940	133.3	939	14.3	925	9.6	960	1.2	950	59.7
25	1041	34.3	1037	83.3	948	0.0	936	0.6	991	11.3	950	0.1	954	111.6	947	1.7	982	0.5	960	1.8
26	1066	67.7	1060	8.4	987	12.6	979	11.1	1013	141.6	993	5.7	983	22.7	989	1.3	996	57.4	982	0.5
27	1130	5.1	1124	22.6	1093	41.5	1121	29.9	1099	96.5	1063	191.7	1094	28.8	1098	58.2	1038	3.5	1037	1.0
28	1146	15.9	1152	2.1	1156	14.0	1151	3.5	1149	15.3	1143	2.0	1139	35.3	1142	21.9	1113	17.7	1083	7.7
29	1157	38.6	1166	14.6	1161	23.8	1160	62.6	1157	1.0	1160	19.8	1153	45.0	1171	21.5	1149	15.4	1148	4.7
30	1189	43.3	1179	43.9	1185	104.8	1188	12.0	1198	6.4	1189	76.0	1185	1.6	1193	114.1	1170	66.5	1171	20.9

Table S2. (continued)

<i>anti-1</i>		<i>syn-1</i>		<i>E,E-2</i>		<i>E,Z-2'</i>		<i>E,Z-2</i>		<i>Z,E-2</i>		<i>Z,Z-2'</i>		<i>Z,Z-2</i>		<i>syn-3</i>		<i>anti-3</i>		
No.	ν/cm^{-1}	Rel.int.	ν/cm^{-1}	Rel.int.	ν/cm^{-1}	rel.int.	ν/cm^{-1}	rel.int.	ν/cm^{-1}	rel.int.	ν/cm^{-1}	rel.int.	ν/cm^{-1}	rel.int.	ν/cm^{-1}	rel.int.	ν/cm^{-1}	rel.int.	ν/cm^{-1}	rel.int.
31	1227	0.5	1276	7.1	1208	84.0	1208	35.7	1233	19.4	1220	252.2	192.2	1234	1214	142.8	1218	4.2	1182	21.5
32	1268	19.4	1314	32.5	1247	311.3	1258	83.1	1289	142.1	1238	234.5	31.9	1264	1269	73.1	1251	7.8	1258	32.9
33	1311	58.3	1331	214.9	1272	262.1	1278	289.3	1314	195.8	1273	172.3	342.5	1273	1274	204.4	1317	16.7	1304	9.8
34	1336	225.5	1354	75.7	1310	1.3	1299	111.3	1381	4.4	1326	4.0	81.4	1294	1371	13.5	1380	46.5	1360	63.5
35	1404	33.4	1395	91.5	1375	18.1	1384	9.0	1404	11.9	1346	41.4	5.9	1387	1387	15.2	1408	43.8	1388	21.9
36	1431	0.6	1432	2.4	1404	1.4	1407	18.5	1441	30.7	1412	5.1	6.4	1401	1421	17.3	1433	78.6	1397	25.5
37	1449	6.8	1461	4.1	1440	2.8	1435	1.3	1443	4.5	1434	2.0	0.4	1430	1437	10.5	1440	21.3	1438	16.7
38	1469	2.0	1473	5.8	1528	9.7	1523	8.0	1522	60.8	1537	6.4	5.2	1531	1531	56.0	1468	47.7	1463	21.8
39	1552	155.1	1551	137.3	1580	97.0	1608	23.2	1572	309.1	1588	171.6	46.2	1614	1578	310.6	1557	49.8	1571	2.2
40	1573	46.9	1573	47.9	1627	55.0	1628	114.1	1609	64.2	1626	171.2	238.2	1628	1626	43.2	1593	51.4	1589	53.4
41	1609	54.8	1604	37.1	1636	76.5	1641	138.1	1626	8.6	1635	26.2	106.1	1639	1634	161.2	1692	249.7	1720	219.9
42	2913	25.4	2923	41.4	3068	14.1	3040	8.8	2497	121.0	3068	15.9	5.7	3046	3060	0.2	2833	102.1	2890	96.7
43	2940	28.3	2990	28.8	3082	17.0	3055	7.0	3046	7.8	3082	17.1	8.0	3055	3073	7.6	3060	5.4	3070	4.3
44	3073	6.3	3071	1.7	3106	7.6	3071	24.4	3063	3.6	3110	6.2	24.4	3072	3076	23.1	3073	9.8	3085	13.1
45	3090	15.9	3083	11.0	3132	1.9	3087	26.2	3071	19.5	3126	3.7	22.8	3087	3091	20.8	3093	16.7	3098	7.4
46	3127	0.8	3094	13.8	3153	2.5	3129	2.2	3092	18.9	3164	2.5	3.8	3122	3125	3.0	3124	1.4	3120	2.1
47	3129	2.6	3126	1.4	3535	117.2	3540	108.4	3131	1.2	3516	132.8	124.7	3524	3317	80.0	3385	144.6	3403	3.7
48	3628	33.4	3571	54.2	3640	138.1	3618	118.9	3536	128.9	3642	139.9	132.9	3630	3516	135.8	3419	4.2	3562	51.7

Table S2. (continued)

<i>cis-5'</i>			<i>cis-5</i>			<i>trans-5'</i>			<i>trans-5</i>			<i>6'</i>			<i>6</i>			
No.	ν/cm^{-1}	rel.int.	ν/cm^{-1}	rel.int.	ν/cm^{-1}	rel.int.	ν/cm^{-1}	rel.int.	ν/cm^{-1}	rel.int.	ν/cm^{-1}	rel.int.	ν/cm^{-1}	rel.int.	ν/cm^{-1}	rel.int.	ν/cm^{-1}	rel.int.
1	89	1.0	71	0.5	66	2.7	77	2.0	78	1.2	59	0.5						
2	107	1.2	114	0.7	113	0.2	110	0.6	102	1.2	112	0.9						
3	153	4.8	147	0.6	151	3.7	146	0.5	157	0.3	132	0.2						
4	240	5.8	243	1.7	273	26.6	247	5.0	222	1.6	205	4.7						
5	305	98.4	347	18.2	279	21.9	301	3.3	251	1.2	254	9.1						
6	355	6.5	356	23.5	326	39.7	349	56.1	278	39.0	282	5.9						
7	368	28.1	384	60.2	378	58.0	378	81.5	304	35.5	311	29.1						
8	417	79.3	404	52.7	399	31.1	395	1.4	343	40.5	337	0.6						
9	444	7.0	451	17.7	420	33.0	421	61.0	360	22.2	356	83.4						
10	482	5.1	498	32.1	511	5.2	494	6.7	440	2.4	456	3.4						
11	522	8.8	539	7.9	515	21.6	527	8.7	460	0.0	464	6.0						
12	537	9.0	544	6.9	546	7.9	546	7.4	541	10.5	528	0.9						
13	540	2.8	555	16.1	556	3.9	570	1.9	556	1.6	542	9.0						
14	612	1.9	615	3.2	622	11.1	634	20.2	630	13.8	621	37.9						
15	715	7.1	718	1.8	697	5.9	696	1.3	659	12.7	636	18.4						
16	738	44.2	736	33.1	721	8.8	715	3.5	693	38.9	678	138.1						
17	743	46.1	740	74.9	744	48.2	744	78.2	721	108.3	743	1.4						
18	776	40.2	789	43.3	753	45.0	792	34.2	734	12.2	757	54.2						
19	799	72.2	814	43.2	805	60.7	803	118.6	759	38.5	796	14.1						
20	844	7.4	844	12.0	840	9.1	831	16.4	848	33.3	817	27.9						
21	861	6.8	860	12.6	868	30.6	861	7.4	874	2.5	871	2.4						
22	911	12.5	893	29.9	911	4.9	893	19.1	941	4.5	944	5.6						
23	915	62.8	898	50.1	945	0.5	913	3.9	968	0.2	968	0.4						
24	929	44.8	914	4.0	956	87.3	924	72.1	1006	100.1	1005	108.1						
25	947	0.2	949	0.2	959	51.0	949	0.3	1040	48.1	1026	39.8						
26	1008	1.9	1006	1.6	1010	2.4	1006	1.5	1058	90.7	1058	82.5						
27	1045	113.9	1042	178.9	1032	124.7	1060	60.4	1077	98.9	1071	88.1						
28	1088	24.4	1088	20.9	1088	39.7	1098	66.2	1135	100.3	1137	90.9						
29	1142	10.3	1142	2.9	1142	9.7	1142	2.8	1146	19.7	1150	27.2						
30	1155	42.2	1153	15.2	1154	65.8	1160	42.1	1152	13.7	1157	43.3						

Table S2. (continued)

<i>cis-5'</i>		<i>cis-5</i>		<i>trans-5'</i>		<i>trans-5</i>		<i>6'</i>		<i>6</i>		
No.	ν/cm^{-1}	Rel.int.	ν/cm^{-1}	Rel.int.	ν/cm^{-1}	rel.int.	ν/cm^{-1}	rel.int.	ν/cm^{-1}	rel.int.	ν/cm^{-1}	rel.int.
31	1177	67.8	1196	10.6	1179	39.8	1201	12.9	1216	45.5	1213	50.1
32	1204	12.1	1228	5.4	1206	1.6	1233	8.8	1261	28.4	1251	28.4
33	1257	2.9	1263	12.9	1258	5.1	1262	1.7	1293	13.6	1295	12.2
34	1316	8.3	1284	20.4	1311	13.6	1283	12.8	1314	71.9	1325	46.7
35	1331	1.7	1328	3.5	1334	8.8	1329	3.8	1387	4.3	1382	4.0
36	1369	57.4	1348	51.3	1384	70.0	1362	57.8	1425	59.9	1425	40.0
37	1402	36.7	1404	100.2	1399	33.9	1403	125.0	1448	44.3	1453	122.3
38	1455	19.1	1452	13.2	1454	23.4	1452	15.4	1453	104.4	1469	3.3
39	1470	4.5	1463	6.4	1470	5.4	1464	8.8	1528	173.2	1543	188.2
40	1599	4.1	1595	3.1	1601	6.3	1597	5.6	1567	12.4	1572	0.6
41	1608	6.8	1606	3.8	1607	6.7	1607	4.2	1596	2.1	1606	8.0
42	2925	56.7	3010	24.9	2910	69.0	2961	38.6	2916	59.1	2917	62.4
43	3067	0.8	3067	0.3	3067	1.1	3067	0.6	3067	2.8	3068	1.0
44	3078	11.9	3078	10.0	3078	12.7	3078	9.5	3079	9.6	3078	12.5
45	3089	20.7	3088	20.2	3090	20.1	3088	19.3	3089	10.6	3089	16.5
46	3100	7.8	3099	7.9	3103	6.4	3099	7.7	3100	9.9	3107	4.3
47	3575	43.7	3562	23.2	3575	50.9	3562	18.0	3435	140.2	3448	126.3
48	3586	23.8	3575	48.0	3580	22.3	3577	45.6	3579	29.2	3572	23.6

Coordinates of optimised structures

B3LYP/6-31G(d)

Neutral species, R=H

syn-1

C	1	-0.218006	-0.836799	0.245432
C	2	-0.114163	0.552465	0.036575
C	3	-1.228987	1.363658	-0.191179
C	4	-2.495413	0.792961	-0.238199
C	5	-2.635955	-0.581333	-0.038945
C	6	-1.512532	-1.370713	0.202864
C	7	0.950789	-1.779244	0.508750
H	8	1.605438	-1.362643	1.285563
O	9	1.671899	-2.104243	-0.664414
H	10	0.545358	-2.722104	0.887338
N	11	1.185439	1.243193	0.056474
O	12	2.215267	0.582144	-0.133479
O	13	1.189334	2.455300	0.252259
H	14	-1.081903	2.427315	-0.331196
H	15	-3.363061	1.417434	-0.427227
H	16	-3.620328	-1.039794	-0.069849
H	17	-1.633029	-2.438479	0.363658
H	18	2.163047	-1.295666	-0.890327

anti-1

C	1	-0.715967	-0.157887	0.000035
C	2	0.639926	0.230032	0.000015
C	3	1.031233	1.572046	0.000011
C	4	0.067778	2.572105	0.000039
C	5	-1.282322	2.218102	0.000060
C	6	-1.660983	0.876946	0.000054
C	7	-1.204620	-1.593487	0.000025
H	8	-0.804127	-2.116867	-0.878501
O	9	-2.626944	-1.594579	-0.000265
H	10	-0.804481	-2.116732	0.878795
N	11	1.726939	-0.760919	0.000010
O	12	1.424236	-1.958200	0.000375
O	13	2.887576	-0.351839	-0.000349
H	14	2.089094	1.801271	-0.000013
H	15	0.369314	3.615059	0.000046
H	16	-2.047978	2.989098	0.000080
H	17	-2.708498	0.604297	0.000054
H	18	-2.911104	-2.519892	-0.000053

E,E-2

C	1	-0.787491	-0.294063	0.000041
C	2	0.573170	0.261720	-0.000028
C	3	0.756374	1.692181	0.000016
C	4	-0.317859	2.524543	0.000120
C	5	-1.660598	2.006303	0.000190
C	6	-1.876392	0.666803	0.000152
C	7	-1.065197	-1.635898	0.000008
H	8	3.475861	-0.690276	-0.000255
O	9	-2.356604	-2.060909	0.000077
H	10	-0.288451	-2.386760	-0.000072
N	11	1.633864	-0.539086	-0.000131
O	12	1.677212	-1.801593	-0.000183
O	13	2.902709	0.100680	-0.000192
H	14	1.766071	2.080150	-0.000037
H	15	-0.160773	3.599481	0.000152
H	16	-2.499007	2.696683	0.000273
H	17	-2.884509	0.267994	0.000204
H	18	-2.364831	-3.028635	0.000041

Z,E-2

C	1	-0.732087	-0.353295	0.000065
C	2	0.571499	0.334637	-0.000051
C	3	0.608715	1.779865	0.000019
C	4	-0.533658	2.511017	0.000195
C	5	-1.820644	1.864298	0.000318
C	6	-1.905060	0.512028	0.000255
C	7	-0.929017	-1.707533	0.000008
H	8	2.758971	-1.808727	-0.000389
O	9	-2.194626	-2.212068	0.000132
H	10	-0.124367	-2.426569	-0.000132
N	11	1.769641	-0.251634	-0.000218
O	12	1.790828	-1.669095	-0.000297
O	13	2.909973	0.281201	-0.000318
H	14	1.587019	2.242998	-0.000074
H	15	-0.477570	3.595840	0.000245
H	16	-2.723428	2.468198	0.000461
H	17	-2.871359	0.021572	0.000348
H	18	-2.144640	-3.178274	0.000071

E,Z-2'

C	1	0.368393	0.940942	0.104769
C	2	0.000918	-0.468876	-0.073860
C	3	1.035758	-1.429632	-0.375894
C	4	2.342467	-1.080913	-0.234700
C	5	2.719329	0.239889	0.204217
C	6	1.773584	1.198580	0.371052
C	7	-0.452704	2.018761	-0.068635
H	8	-2.411693	-2.309491	0.228567
O	9	-1.677058	1.947886	-0.628365
H	10	-0.085408	3.014412	0.176992
N	11	-1.243581	-0.871943	0.179281
O	12	-2.211190	-0.242389	0.654541
O	13	-1.495969	-2.247397	-0.105502
H	14	0.748895	-2.433617	-0.659800
H	15	3.117480	-1.815714	-0.433573
H	16	3.767983	0.468401	0.370011
H	17	2.057507	2.213421	0.640822
H	18	-2.142436	2.788888	-0.505065

E,Z-2

C	1	0.405865	0.926925	0.079691
C	2	0.009496	-0.480196	-0.016499
C	3	1.031021	-1.477163	-0.216047
C	4	2.346990	-1.134039	-0.130543
C	5	2.759146	0.214671	0.130251
C	6	1.819003	1.192523	0.229537
C	7	-0.411647	2.034010	-0.094104
H	8	-2.477112	-2.231033	0.197488
O	9	-1.678044	2.088879	-0.425937
H	10	0.046786	3.018621	-0.002608
N	11	-1.258599	-0.848402	0.112837
O	12	-2.276706	-0.141112	0.495970
O	13	-1.566043	-2.193528	-0.153073
H	14	0.727974	-2.502246	-0.382042
H	15	3.102000	-1.906655	-0.248304
H	16	3.814943	0.449423	0.218927
H	17	2.117655	2.227311	0.377868
H	18	-2.114954	1.189102	-0.180582

<i>Z,Z-2'</i>				
C	1	0.309686	0.919280	0.111418
C	2	0.034908	-0.511989	-0.082583
C	3	1.133916	-1.396153	-0.401350
C	4	2.415071	-0.977240	-0.239283
C	5	2.703828	0.355771	0.233866
C	6	1.699786	1.249566	0.406712
C	7	-0.527985	1.974268	-0.105552
H	8	-2.882337	-0.961787	0.703260
O	9	-1.770056	1.886928	-0.631612
H	10	-0.165136	2.979298	0.102590
N	11	-1.148409	-1.093397	0.108840
O	12	-2.155707	-0.307463	0.694795
O	13	-1.468141	-2.287835	-0.115140
H	14	0.890355	-2.408660	-0.698475
H	15	3.235100	-1.660368	-0.441538
H	16	3.733553	0.644965	0.422345
H	17	1.919852	2.272658	0.703251
H	18	-2.156560	2.773622	-0.677023

<i>Z,Z-2</i>				
C	1	0.335147	0.919115	0.082063
C	2	0.038007	-0.518476	-0.044472
C	3	1.132161	-1.437590	-0.275710
C	4	2.420268	-1.025751	-0.157878
C	5	2.736737	0.338850	0.173856
C	6	1.739822	1.250256	0.286417
C	7	-0.487040	2.006618	-0.110670
H	8	-2.967079	-0.899010	0.496530
O	9	-1.767279	2.086484	-0.462553
H	10	-0.047496	2.996155	-0.013526
N	11	-1.156015	-1.093023	0.073363
O	12	-2.238980	-0.245833	0.526669
O	13	-1.498038	-2.287148	-0.112927
H	14	0.874401	-2.467775	-0.485982
H	15	3.224604	-1.742040	-0.300144
H	16	3.772526	0.635856	0.305090
H	17	1.974758	2.292560	0.486248
H	18	-2.195852	1.209257	-0.332912

<i>syn-3</i>				
C	1	0.412473	0.907705	-0.000685
C	2	0.022547	-0.459022	-0.093456
C	3	1.008155	-1.451654	-0.125021
C	4	2.355358	-1.117221	0.002674
C	5	2.752619	0.213969	0.144501
C	6	1.780781	1.206412	0.127298
C	7	-0.477963	2.073753	-0.140001
H	8	-1.538704	-2.447970	0.636831
O	9	-1.689632	2.098498	-0.315993
H	10	0.073218	3.036077	-0.113314
N	11	-1.347092	-0.779095	-0.267099
O	12	-2.138332	-0.235772	0.776484
O	13	-1.603156	-2.150569	-0.296443
H	14	0.707697	-2.483147	-0.256278
H	15	3.099435	-1.909262	-0.006072
H	16	3.802180	0.471436	0.245957
H	17	2.074219	2.251361	0.199285
H	18	-2.463263	0.594268	0.359039

<i>anti-3</i>				
C	1	-0.759607	1.909571	-0.267138
C	2	-0.750362	0.433112	-0.079179
C	3	-0.924924	-2.358829	0.053520
C	4	0.419532	-0.357300	-0.154996
C	5	-1.984689	-0.202610	0.107079
C	6	-2.080990	-1.588510	0.182232
C	7	0.320213	-1.750907	-0.114604
N	8	1.695369	0.279265	-0.345695
O	9	1.850029	1.232433	0.715915
O	10	2.765752	-0.623305	-0.235492
O	11	-1.739933	2.601372	-0.061930
H	12	0.172714	2.358814	-0.650504
H	13	-0.983712	-3.443374	0.085093
H	14	-2.864674	0.429427	0.173365
H	15	-3.047139	-2.064558	0.320572
H	16	1.210822	-2.354764	-0.232887
H	17	2.462318	1.880721	0.324511
H	18	2.740271	-0.952283	0.690288

<i>cis-5'</i>				
C	1	0.218363	-0.721897	-0.231511
C	2	0.251707	0.663990	-0.239928
C	3	1.429564	1.378677	-0.053865
C	4	2.602844	0.642581	0.122789
C	5	2.584051	-0.758848	0.123179
C	6	1.384555	-1.455732	-0.045877
C	7	-1.213176	-1.144607	-0.376440
H	8	-2.094444	2.468559	0.503853
O	9	-1.656928	-1.706273	0.830276
H	10	-1.408299	-1.822476	-1.218432
N	11	-1.047216	1.229461	-0.464899
O	12	-1.881955	0.076329	-0.742871
O	13	-1.457588	1.791274	0.789192
H	14	1.429290	2.463481	-0.047183
H	15	3.544864	1.165820	0.261115
H	16	3.511074	-1.307792	0.261510
H	17	1.362716	-2.541394	-0.023026
H	18	-2.590370	-1.948053	0.713593

<i>cis-5</i>				
H	1	1.402869	1.880895	-1.165431
C	2	-0.223012	0.718906	-0.231499
C	3	-2.610813	-0.644981	0.123326
C	4	-0.266523	-0.666838	-0.262431
C	5	-1.384345	1.453773	-0.017744
C	6	-2.584588	0.755881	0.150643
C	7	-1.441216	-1.383302	-0.077043
N	8	1.046899	-1.221468	-0.476864
H	9	-1.360911	2.539264	0.019612
H	10	-3.508899	1.305387	0.304690
H	11	-1.444969	-2.468178	-0.091247
H	12	-3.554531	-1.165798	0.258386
O	13	1.834346	-0.086740	-0.867158
O	14	1.482571	-1.603358	0.857246
H	15	2.211765	-2.216453	0.659305
O	16	1.805833	1.631434	0.776264
H	17	1.694962	0.947306	1.459625
C	18	1.218734	1.132756	-0.391536

<i>trans-5'</i>				
C	1	0.188067	-0.712380	-0.226603
C	2	0.199957	0.613684	0.177829
C	3	1.382408	1.309449	0.403977
C	4	2.579226	0.616399	0.208984
C	5	2.581244	-0.727287	-0.187149
C	6	1.378697	-1.406749	-0.403653
C	7	-1.244324	-1.145439	-0.340120
H	8	-1.973908	2.752495	0.009300
O	9	-1.529019	-2.050348	0.702068
H	10	-1.526002	-1.578367	-1.310696
N	11	-1.124803	1.115029	0.376051
O	12	-1.978923	0.072505	-0.223294
O	13	-1.283276	2.251890	-0.457420
H	14	1.367356	2.351179	0.705199
H	15	3.523335	1.130764	0.365435
H	16	3.525727	-1.245222	-0.326409
H	17	1.375367	-2.449830	-0.706119
H	18	-2.480166	-2.244656	0.660512

<i>trans-5</i>				
C	1	-0.139976	-0.657373	0.198699
C	2	-0.254417	0.655686	-0.227719
C	3	-1.484038	1.266021	-0.438053
C	4	-2.626525	0.492801	-0.213510
C	5	-2.525685	-0.840080	0.206460
C	6	-1.275373	-1.429386	0.419735
C	7	1.324631	-0.989862	0.320032
H	8	1.883925	2.743479	0.413881
O	9	1.747219	-2.135306	-0.351971
H	10	1.663082	-1.122282	1.353764
N	11	1.036705	1.264475	-0.416520
O	12	1.961070	0.169983	-0.275096
O	13	1.212140	2.117856	0.734918
H	14	-1.548104	2.299756	-0.761111
H	15	-3.607545	0.932240	-0.370548
H	16	-3.429299	-1.421679	0.365338
H	17	-1.190945	-2.462890	0.743641
H	18	1.496813	-2.027054	-1.286009

6'				
C	1	0.081233	-0.567921	-0.039740
C	2	0.434864	0.806927	0.059087
C	3	1.783650	1.194965	0.114922
C	4	2.805770	0.257212	0.014795
C	5	2.470024	-1.089593	-0.107325
C	6	1.127066	-1.485265	-0.119875
C	7	-1.341775	-1.118399	0.003346
H	8	-2.174866	0.254026	-1.012815
O	9	-1.882852	-0.740785	1.254822
H	10	-1.283697	-2.212567	-0.080049
N	11	-0.417965	1.952394	0.114530
O	12	-2.146381	-0.724324	-1.068767
O	13	-1.586894	1.818991	-0.233165
H	14	1.992022	2.255138	0.219860
H	15	3.845000	0.570170	0.041077
H	16	3.249883	-1.843185	-0.174739
H	17	0.889246	-2.543706	-0.183077
H	18	-2.827818	-0.965254	1.213656

6				
C	1	1.781158	0.908539	0.052748
C	2	0.838720	-1.715388	-0.125335
C	3	0.405393	0.645077	-0.021114
C	4	2.684083	-0.144939	0.034776
C	5	2.209200	-1.459284	-0.055153
C	6	-0.088826	-0.672916	-0.114117
N	7	-0.563923	1.702171	-0.055401
C	8	-1.580490	-0.994378	-0.133987
O	9	-0.137603	2.826273	0.158651
O	10	-2.021396	-0.844314	1.204888
O	11	-2.334092	-0.227189	-1.027044
H	12	2.103597	1.942414	0.113782
H	13	0.484328	-2.740834	-0.186117
H	14	3.751743	0.048020	0.084510
H	15	2.911658	-2.288090	-0.072467
H	16	-1.710587	-2.031712	-0.472878
H	17	-2.982972	-0.989100	1.185636
H	18	-2.160994	0.705677	-0.783527

TS[E,E-2'-cis-5']				
C	1	0.888795	1.623218	-0.260755
C	2	-0.214917	0.729925	-0.209947
C	3	-2.354244	-1.100539	-0.003244
C	4	-0.000317	-0.679428	-0.270140
C	5	-1.542256	1.183052	0.031473
C	6	-2.589311	0.293176	0.108878
C	7	-1.078927	-1.587494	-0.181679
N	8	1.309630	-1.077274	-0.276359
O	9	2.199186	-0.140833	-0.318699
O	10	0.777458	2.744893	0.487276
H	11	1.596542	1.663961	-1.072810
H	12	-3.188034	-1.793235	0.069878
H	13	-1.716587	2.251945	0.103465
H	14	-3.603235	0.658620	0.243368
H	15	-0.872788	-2.650627	-0.218521
H	16	1.475655	3.369130	0.234198
O	17	1.537035	-2.132520	0.695480
H	18	2.378671	-2.502646	0.374963

TS[E,Z-2'-trans-5']				
C	1	0.184327	-0.878024	-0.144709
C	2	0.120841	0.499183	0.247610
C	3	1.298350	1.235657	0.511363
C	4	2.520656	0.638740	0.293748
C	5	2.608387	-0.681528	-0.213659
C	6	1.462992	-1.412774	-0.447535
C	7	-1.022397	-1.602776	-0.303925
H	8	-1.896847	2.761192	-0.220997
O	9	-1.798035	-1.844313	0.772069
H	10	-1.145952	-2.293448	-1.142541
N	11	-1.110321	1.073834	0.116178
O	12	-2.091096	0.351537	-0.292419
O	13	-1.018863	2.404318	-0.445030
H	14	1.216378	2.268051	0.829048
H	15	3.430900	1.200370	0.484674
H	16	3.582743	-1.126309	-0.392596
H	17	1.530512	-2.440859	-0.793177
H	18	-2.720468	-1.969041	0.488018

TS[E,Z-2-trans-5]				
H	1	-1.324896	2.293298	-0.694611
C	2	-1.365473	1.240719	-0.440522
C	3	-1.413903	-1.451540	0.371237
C	4	-0.165973	0.538521	-0.229591
C	5	-2.567149	0.581614	-0.259954
C	6	-2.595735	-0.765571	0.157654
C	7	-0.164621	-0.834208	0.121790
N	8	1.079383	1.146725	-0.213291
H	9	-3.499854	1.117299	-0.412629
H	10	-3.547840	-1.267643	0.301295
C	11	1.065373	-1.562588	0.337794
H	12	-1.436236	-2.493966	0.677759
O	13	2.053335	0.342279	0.132187
O	14	1.018028	2.377962	0.546066
O	15	1.978520	-1.926808	-0.565740
H	16	1.053978	-2.275225	1.165378
H	17	2.246484	-1.081698	-1.003626
H	18	1.798505	2.851718	0.208922

TS[E,Z-2-syn-3]				
H	1	0.720187	-2.509217	-0.329463
C	2	1.028956	-1.482538	-0.183295
C	3	1.829249	1.189103	0.209952
C	4	0.020413	-0.479919	0.005561
C	5	2.351460	-1.139788	-0.110800
C	6	2.771630	0.204499	0.119845
C	7	0.426007	0.914762	0.084003
N	8	-1.260726	-0.823495	0.128173
H	9	3.101196	-1.919634	-0.216268
H	10	3.828827	0.438066	0.191614
C	11	-0.426295	2.011300	-0.121712
H	12	2.129092	2.227339	0.330772
O	13	-2.254589	-0.070040	0.567174
O	14	-1.637960	-2.113982	-0.252613
O	15	-1.667450	1.994365	-0.456824
H	16	0.021509	3.007053	-0.043617
H	17	-2.117919	1.018906	-0.064425
H	18	-2.386336	-2.285304	0.350959

TS[cis-5-trans-5]				
C	1	1.301223	1.462530	0.184140
C	2	1.536312	-1.336456	-0.246019
C	3	0.179236	0.659579	-0.046836
C	4	2.545382	0.827648	0.179133
C	5	2.677266	-0.549332	-0.038887
C	6	0.293389	-0.726733	-0.251576
N	7	-1.138813	0.982797	-0.114526
C	8	-1.100319	-1.292392	-0.329379
O	9	-1.774878	2.159194	0.056705
O	10	-1.942393	-0.128634	-0.514173
O	11	-1.387318	-1.975847	0.867117
H	12	1.202619	2.530343	0.345448
H	13	1.622371	-2.410471	-0.388702
H	14	3.436224	1.428539	0.343837
H	15	3.661034	-1.007845	-0.037110
H	16	-1.315124	-1.924982	-1.199318
H	17	-2.116832	2.156880	0.976444
H	18	-2.276821	-2.358807	0.780428

Neutral species, R=Me				
syn-1				
C	1	1.757610	-0.236334	-0.219593
C	2	0.406305	0.482402	-0.078860
C	3	-2.072278	1.863471	0.183452
C	4	-0.833104	-0.189287	-0.039348
C	5	0.342301	1.878483	0.025774
C	6	-0.864886	2.562391	0.163197
C	7	-2.055504	0.479088	0.070248
N	8	-0.928659	-1.657123	-0.108904
H	9	1.264318	2.447251	-0.007232
H	10	-0.860142	3.645452	0.248647
H	11	-2.970430	-0.100593	0.073720
H	12	-3.017110	2.388262	0.285284
O	13	0.007443	-2.337564	0.332483
O	14	-1.951926	-2.143017	-0.582312
O	15	2.186249	-0.728384	1.044927
C	16	2.886754	0.639882	-0.752929
H	17	1.620806	-1.069556	-0.921547
H	18	1.577397	-1.457599	1.255452
H	19	3.770491	0.012736	-0.899296
H	20	2.622624	1.103180	-1.709214
H	21	3.155345	1.421871	-0.035922

anti-1				
C	1	-1.744067	-0.317502	-0.249380
C	2	-0.421827	0.423497	-0.091572
C	3	1.948361	1.961729	0.209324
C	4	0.851659	-0.173770	-0.019807
C	5	-0.456250	1.823839	-0.015905
C	6	0.700124	2.583670	0.140778
C	7	2.022887	0.578576	0.116884
N	8	1.041231	-1.632338	-0.096132
O	9	0.088221	-2.365685	0.182504
O	10	2.151295	-2.049227	-0.424888
O	11	-2.622215	0.559315	-0.964906
C	12	-2.346450	-0.689474	1.113798
H	13	-1.581183	-1.231394	-0.828986
H	14	2.855244	2.546652	0.328426
H	15	-1.421073	2.308901	-0.102315
H	16	0.625650	3.665883	0.202862
H	17	2.971879	0.058313	0.148902
H	18	-3.491122	0.130068	-0.986330
H	19	-1.680317	-1.352531	1.669566
H	20	-3.300791	-1.213281	0.971751
H	21	-2.531927	0.215146	1.702638

<i>E,E-2</i>				
C	1	-0.534427	0.558041	-0.094962
C	2	0.729438	-0.164013	0.080049
C	3	1.916574	0.585120	0.422167
C	4	1.917295	1.938842	0.284148
C	5	0.751641	2.642423	-0.180804
C	6	-0.418857	1.977831	-0.371310
C	7	-1.774424	-0.002256	0.123027
H	8	1.958674	-2.914193	-0.378265
O	9	-2.860329	0.742676	-0.233418
C	10	-2.040008	-1.308863	0.793546
N	11	0.825817	-1.458716	-0.226094
O	12	-0.000419	-2.232538	-0.782189
O	13	2.087182	-2.053565	0.065570
H	14	2.808542	0.049016	0.717791
H	15	2.822916	2.496943	0.505942
H	16	0.804423	3.715308	-0.341180
H	17	-1.319625	2.510912	-0.653085
H	18	-3.664759	0.294310	0.066909
H	19	-3.046250	-1.322767	1.231785
H	20	-1.318173	-1.482066	1.598500
H	21	-1.921328	-2.151781	0.099385

<i>E,Z-2'</i>				
C	1	-0.540902	0.543388	-0.057691
C	2	0.750169	-0.146731	0.086606
C	3	1.936022	0.624003	0.377314
C	4	1.907017	1.975983	0.235796
C	5	0.708795	2.651037	-0.191986
C	6	-0.455206	1.964774	-0.337790
C	7	-1.747913	-0.073831	0.173190
H	8	1.977550	-2.904366	-0.352782
O	9	-1.748141	-1.226439	0.888276
C	10	-3.102858	0.449273	-0.203663
N	11	0.852343	-1.439958	-0.220035
O	12	-0.001229	-2.234171	-0.673389
O	13	2.146637	-2.003395	-0.016051
H	14	2.844306	0.105203	0.654761
H	15	2.804812	2.556431	0.428858
H	16	0.733254	3.723855	-0.359848
H	17	-1.365810	2.501635	-0.584098
H	18	-2.460089	-1.815737	0.586914
H	19	-3.671820	-0.340903	-0.716782
H	20	-3.054606	1.302195	-0.881913
H	21	-3.682875	0.736043	0.683788

<i>E,Z-2</i>				
C	1	-0.679594	0.291500	0.101394
C	2	0.773154	0.138277	-0.014193
C	3	1.582095	1.304346	-0.261637
C	4	1.035010	2.549169	-0.164487
C	5	-0.346014	2.730585	0.159527
C	6	-1.156524	1.641573	0.283826
C	7	-1.617748	-0.729588	-0.117518
H	8	2.950499	-1.984373	0.234349
O	9	-1.318846	-1.950082	-0.497602
C	10	-3.107561	-0.495554	-0.033247
N	11	1.366304	-1.039478	0.148604
O	12	0.850994	-2.151970	0.590923
O	13	2.727780	-1.133525	-0.190061
H	14	2.635893	1.168140	-0.464581
H	15	1.668177	3.419424	-0.315424
H	16	-0.747924	3.732073	0.276146
H	17	-2.212867	1.789427	0.478461
H	18	-0.366516	-2.210302	-0.146083
H	19	-3.611728	-1.458183	-0.133738
H	20	-3.400212	-0.041030	0.919224
H	21	-3.455774	0.163943	-0.836661

<i>syn-3</i>				
C	1	-0.482401	0.520059	0.057210
C	2	0.797344	-0.095586	0.135774
C	3	1.948030	0.710652	0.066706
C	4	1.866202	2.089249	-0.034845
C	5	0.614040	2.715063	-0.033312
C	6	-0.528385	1.934541	0.022077
C	7	-1.769391	-0.197931	-0.156085
H	8	2.329107	-2.693649	-0.327100
O	9	-1.826879	-1.339641	-0.616841
C	10	-3.079857	0.521332	0.126555
N	11	1.096432	-1.463523	0.420487
O	12	0.063140	-2.289122	0.810852
O	13	1.755222	-2.020794	-0.733390
H	14	2.912004	0.217776	0.126138
H	15	2.776593	2.680183	-0.083605
H	16	0.534773	3.796848	-0.081812
H	17	-1.494227	2.425845	-0.005635
H	18	-0.617075	-2.249530	0.087627
H	19	-3.873706	-0.227243	0.147790
H	20	-3.057248	1.068259	1.074265
H	21	-3.310598	1.238341	-0.670520

<i>cis-5'</i>				
C	1	0.182885	-0.613082	-0.007387
C	2	0.612788	0.677020	-0.275701
C	3	1.958908	1.021743	-0.299579
C	4	2.884705	0.003906	-0.059637
C	5	2.464057	-1.306271	0.203650
C	6	1.103233	-1.624844	0.240114
C	7	-1.323785	-0.606447	0.009363
H	8	-1.018588	3.195826	0.275625
O	9	-1.737334	-0.728429	1.351543
C	10	-2.019431	-1.626307	-0.888739
N	11	-0.485870	1.567320	-0.523038
O	12	-1.636862	0.693837	-0.549274
O	13	-0.582845	2.406338	0.639455
H	14	2.270232	2.042147	-0.496765
H	15	3.946595	0.232687	-0.078633
H	16	3.203317	-2.080985	0.386023
H	17	0.775542	-2.635554	0.466023
H	18	-2.703360	-0.621454	1.365299
H	19	-3.100272	-1.441431	-0.894641
H	20	-1.841185	-2.637905	-0.511526
H	21	-1.655028	-1.552855	-1.916424

<i>trans-5'</i>				
C	1	0.200794	-0.603295	-0.011411
C	2	0.606787	0.696125	-0.267286
C	3	1.943764	1.072167	-0.261733
C	4	2.887339	0.075135	-0.000714
C	5	2.490846	-1.245703	0.244708
C	6	1.137354	-1.597689	0.243204
C	7	-1.302751	-0.652707	-0.082313
H	8	-1.168318	3.100954	0.372269
O	9	-1.690573	-1.624404	-1.014346
C	10	-2.010186	-0.832541	1.260445
N	11	-0.512724	1.562917	-0.529771
O	12	-1.630031	0.665564	-0.621979
O	13	-0.676759	2.325821	0.693392
H	14	2.235660	2.099248	-0.454325
H	15	3.943925	0.328073	0.006341
H	16	3.244147	-2.005545	0.432853
H	17	0.825970	-2.621854	0.426863
H	18	-2.661630	-1.629752	-1.045691
H	19	-3.095910	-0.759092	1.119425
H	20	-1.704045	-0.045381	1.953911
H	21	-1.775514	-1.811866	1.690809

<i>trans-5</i>				
C	1	-0.202100	-0.597674	-0.002680
C	2	-0.603685	0.702808	-0.260614
C	3	-1.938381	1.085938	-0.258334
C	4	-2.887224	0.092514	0.000180
C	5	-2.497269	-1.230105	0.247450
C	6	-1.144932	-1.587838	0.251033
C	7	1.307716	-0.660137	-0.073757
H	8	1.225448	3.067145	0.396871
O	9	1.805282	-1.629757	-0.951419
C	10	2.009649	-0.855012	1.262939
N	11	0.524584	1.560037	-0.522367
O	12	1.627416	0.651930	-0.643337
O	13	0.709484	2.303629	0.707660
H	14	-2.225656	2.114434	-0.450585
H	15	-3.942638	0.350049	0.004416
H	16	-3.254574	-1.986043	0.435161
H	17	-0.837974	-2.612690	0.440917
H	18	1.406999	-1.457971	-1.821672
H	19	3.091249	-0.806371	1.107417
H	20	1.757181	-1.831802	1.688089
H	21	1.707777	-0.066383	1.955422

TS[E,E-2- <i>cis-5'</i>]				
C	1	0.109043	-0.678980	0.034518
C	2	-0.642419	0.525570	0.230004
C	3	-2.053557	0.489153	0.360922
C	4	-2.712638	-0.709875	0.230409
C	5	-1.999410	-1.903995	-0.052323
C	6	-0.629641	-1.878764	-0.174205
C	7	1.529434	-0.663792	-0.044813
H	8	-0.185024	3.486836	-0.431216
O	9	2.041875	-1.534470	-0.950223
C	10	2.470926	-0.269485	1.057231
N	11	0.049218	1.689599	0.102572
O	12	1.314793	1.646414	-0.125745
O	13	-0.699046	2.685116	-0.635172
H	14	-2.586650	1.419670	0.513898
H	15	-3.794880	-0.739382	0.322619
H	16	-2.536331	-2.842854	-0.151132
H	17	-0.075806	-2.792051	-0.367005
H	18	2.994782	-1.642279	-0.792464
H	19	3.318205	0.313341	0.678725
H	20	2.856133	-1.189726	1.526452
H	21	1.973639	0.323785	1.820778

TS[E,Z-2-trans-5]				
C	1	0.090557	-0.650015	-0.079981
C	2	-0.676168	0.535804	-0.214184
C	3	-2.081494	0.498229	-0.259919
C	4	-2.729819	-0.716414	-0.141978
C	5	-1.995537	-1.904797	0.044049
C	6	-0.613709	-1.865197	0.099738
C	7	1.546120	-0.632719	-0.058090
H	8	-0.232543	3.498910	0.434828
O	9	2.309247	-0.298684	-1.107212
C	10	2.290897	-1.497661	0.916050
N	11	0.037290	1.724677	-0.184200
O	12	1.328255	1.564829	-0.011129
O	13	-0.578607	2.646205	0.751300
H	14	-2.628242	1.429739	-0.346278
H	15	-3.815290	-0.750869	-0.170919
H	16	-2.513303	-2.855692	0.128657
H	17	-0.054318	-2.788471	0.220373
H	18	2.014396	0.624331	-1.328651
H	19	3.172175	-0.948842	1.263657
H	20	2.660439	-2.404084	0.415787
H	21	1.679421	-1.779945	1.774166

B3LYP/6-31+G(d)

Anionic species, R=H

E-2 ⁻				
C	1	1.220854	-1.525089	0.000004
C	2	0.754626	-0.238563	-0.000001
C	3	-0.031502	2.552458	0.000006
C	4	-0.658818	0.184328	0.000000
C	5	1.719709	0.859599	-0.000007
C	6	1.352509	2.173893	-0.000003
C	7	-0.989248	1.566960	0.000006
N	8	-1.709800	-0.718425	-0.000002
O	9	-1.453126	-1.966292	-0.000001
O	10	-2.920532	-0.310482	-0.000005
O	11	2.611858	-1.754760	-0.000005
H	12	0.586849	-2.396399	0.000005
H	13	-0.317733	3.601985	0.000011
H	14	2.771057	0.589640	-0.000014
H	15	2.122281	2.945996	-0.000007
H	16	-2.045694	1.810606	0.000010
H	17	2.737469	-2.712103	0.000053

cis-5 ⁻				
C	1	-0.072875	-0.621261	-0.254436
C	2	2.645435	-0.027752	0.148473
C	3	0.354981	0.707446	-0.137180
C	4	0.876407	-1.645931	-0.198203
C	5	2.231165	-1.358774	0.000518
C	6	1.708490	1.005147	0.085280
N	7	-0.564703	1.793546	-0.403847
O	8	-2.234967	0.309436	-0.251723
O	9	-1.983500	-1.836197	0.663005
C	10	-1.585027	-0.840952	-0.373670
H	11	3.696873	0.203097	0.314324
H	12	0.535669	-2.677362	-0.261568
H	13	2.958103	-2.167228	0.064748
H	14	2.007148	2.045448	0.187785
H	15	-2.311854	-1.250777	1.368152
H	16	-1.792934	-1.404635	-1.314646
O	17	-0.542975	2.700398	0.444149

TS[E-2-cis-5 ⁻]				
C	1	1.283127	1.239568	0.293302
C	2	-0.055297	0.720703	0.256245
C	3	-2.557109	-0.555586	-0.065681
C	4	-0.160307	-0.718742	0.209084
C	5	-1.229753	1.483330	0.068956
C	6	-2.468593	0.872161	-0.053629
C	7	-1.432137	-1.342262	0.041955
N	8	1.016895	-1.353405	0.101346
H	9	-1.148990	2.568864	0.045711
H	10	-3.371643	1.473254	-0.141032
H	11	-1.473765	-2.425385	-0.015829
H	12	-3.532507	-1.027699	-0.180146
O	13	2.057120	-0.499784	0.292605
O	14	1.204426	-2.514066	-0.455031
H	15	1.877578	1.353657	1.196950
O	16	1.481331	2.334046	-0.564127
H	17	2.308466	2.774536	-0.304037

Z-2 ⁻				
C	1	0.274059	0.943081	0.064243
C	2	0.014707	-0.508431	-0.049143
C	3	1.125234	-1.389973	-0.274100
C	4	2.419577	-0.958415	-0.175348
C	5	2.693440	0.417619	0.160974
C	6	1.667894	1.306048	0.283951
C	7	-0.613234	1.980961	-0.109646
O	8	-1.905284	1.906312	-0.471661
H	9	-0.258980	3.004040	0.022697
N	10	-1.214217	-1.079276	0.117014
O	11	-2.221299	-0.353768	0.538013
O	12	-1.404407	-2.325741	-0.079039
H	13	0.890349	-2.429685	-0.472643
H	14	3.241717	-1.656605	-0.319836
H	15	3.722190	0.747296	0.299355
H	16	1.880801	2.353112	0.499110
H	17	-2.218699	0.977008	-0.151873

trans-5⁻

C	1	0.001428	-0.739207	-0.069208
C	2	2.653953	0.216261	0.082375
C	3	0.271475	0.634502	0.084000
C	4	1.080553	-1.617461	-0.155137
C	5	2.401864	-1.148897	-0.083995
C	6	1.581894	1.113427	0.163124
C	7	-1.472488	-1.127976	-0.264858
N	8	-0.854380	1.516326	0.281224
O	9	-2.062293	-0.264106	-1.069652
O	10	-0.692355	2.660060	-0.157923
O	11	-2.088275	-1.190596	1.090165
H	12	-1.518415	-2.197853	-0.582990
H	13	3.677355	0.582422	0.146044
H	14	0.885975	-2.679573	-0.298959
H	15	3.232169	-1.849133	-0.167912
H	16	1.742993	2.179737	0.299167
H	17	-2.408105	-0.276647	1.197561

TS[Z-2-*trans-5⁻*]

C	1	-1.164486	-1.382567	-0.300914
C	2	0.150774	-0.828713	-0.111583
C	3	2.578311	0.552283	0.251606
C	4	0.164481	0.582609	0.187528
C	5	1.373391	-1.471045	-0.367666
C	6	2.583856	-0.811923	-0.166670
C	7	1.403791	1.256842	0.413205
N	8	-1.005192	1.191897	-0.045718
H	9	1.365798	-2.517330	-0.674817
H	10	3.526836	-1.336296	-0.304957
H	11	1.390761	2.310383	0.673245
H	12	3.528804	1.056484	0.425498
O	13	-2.005974	0.303697	-0.335582
O	14	-1.181463	2.456278	-0.285504
O	15	-2.017042	-1.786971	0.725514
H	16	-2.388635	-0.944738	1.068577
H	17	-1.292098	-2.080728	-1.135992

syn-3⁻

C	1	0.319164	0.921604	0.094814
C	2	-0.010059	-0.507135	-0.035228
C	3	1.078905	-1.425445	-0.292834
C	4	2.380558	-1.027377	-0.164388
C	5	2.714786	0.325414	0.183376
C	6	1.702675	1.246202	0.287437
C	7	-0.556690	2.009545	-0.128423
O	8	-1.763847	1.981308	-0.525483
H	9	-0.103444	3.005946	0.040122
N	10	-1.229527	-1.040467	0.094089
O	11	-2.275734	-0.250574	0.579400
O	12	-1.525818	-2.271029	-0.098013
H	13	0.815388	-2.449561	-0.530548
H	14	3.177541	-1.752991	-0.323233
H	15	3.754155	0.620857	0.308983
H	16	1.943787	2.294772	0.465085
H	17	-2.233581	0.629758	0.065217

anti-3⁻

C	1	-0.922218	-1.875764	-0.000315
C	2	-0.775315	-0.427013	-0.000159
C	3	-0.736138	2.414458	0.000095
C	4	0.497549	0.290785	0.000104
C	5	-1.963404	0.345536	-0.000273
C	6	-1.981609	1.726888	-0.000156
C	7	0.457910	1.736419	0.000221
N	8	1.674911	-0.325282	0.000244
H	9	-2.890527	-0.222913	-0.000468
H	10	-2.920086	2.276976	-0.000254
H	11	1.397265	2.275218	0.000414
H	12	-0.718970	3.504501	0.000189
O	13	2.850677	0.534920	0.000492
O	14	1.971536	-1.588870	0.000172
H	15	0.010438	-2.454807	-0.000224
O	16	-2.020098	-2.470415	-0.000540
H	17	3.519931	-0.174941	0.000533

TS[Z-2-*syn-3⁻*]

C	1	0.304133	0.937338	0.071010
C	2	0.007981	-0.504614	-0.039285
C	3	1.104485	-1.409934	-0.270363
C	4	2.402150	-0.994525	-0.163532
C	5	2.708048	0.376846	0.163138
C	6	1.694178	1.284727	0.273840
C	7	-0.595778	1.974762	-0.126493
O	8	-1.854996	1.862214	-0.485712
H	9	-0.231484	3.000155	0.007791
N	10	-1.223493	-1.038702	0.112861
O	11	-2.232426	-0.263351	0.547105
O	12	-1.477746	-2.275402	-0.082034
H	13	0.853668	-2.444449	-0.476589
H	14	3.212410	-1.707301	-0.307731
H	15	3.743689	0.687405	0.289625
H	16	1.922679	2.333509	0.464654
H	17	-2.166347	0.826303	-0.052545

6⁻

C	1	0.015952	-0.550173	-0.123325
C	2	0.384086	0.833042	0.004508
C	3	1.750988	1.205518	0.088936
C	4	2.772519	0.274944	0.020805
C	5	2.426382	-1.081288	-0.132776
C	6	1.093453	-1.463558	-0.193990
C	7	-1.383962	-1.186705	-0.001588
H	8	-2.494245	0.282150	-0.574600
O	9	-1.673177	-1.094470	1.284788
H	10	-1.292274	-2.228010	-0.400825
N	11	-0.421645	1.989982	0.061586
O	12	-2.354130	-0.619079	-0.922391
O	13	-1.653516	1.880015	-0.013922
H	14	1.959909	2.266662	0.200937
H	15	3.814114	0.582881	0.079354
H	16	3.208068	-1.836850	-0.206712
H	17	0.846019	-2.519112	-0.292469

6^-				
C	1	1.766183	0.863002	0.063087
C	2	0.748914	-1.723008	-0.181621
C	3	0.369558	0.654812	-0.034479
C	4	2.638956	-0.208823	0.022431
C	5	2.117733	-1.515820	-0.109150
C	6	-0.176497	-0.654929	-0.142261
N	7	-0.533389	1.743206	-0.055376
C	8	-1.668624	-1.010448	-0.022029
O	9	-0.042541	2.867683	0.130995
O	10	-1.928791	-0.927938	1.271272
O	11	-2.501804	-0.195022	-0.903166
H	12	2.123623	1.884198	0.154984
H	13	0.354037	-2.734483	-0.260033
H	14	3.714100	-0.050566	0.083359
H	15	2.798306	-2.365515	-0.154487
H	16	-1.804743	-2.023087	-0.481837
H	17	-2.443844	0.700519	-0.523026

OH^-				
O	1	0.000000	0.000000	0.108292
H	2	0.000000	0.000000	-0.866333

H_2O				
O	1	-0.000000	0.117279	0.000000
H	2	0.771181	-0.469188	0.000000
H	3	-0.771181	-0.469040	0.000000

o-NBAL in 0.1 M HCl

o-nitrobenzyl alcohol				H ₂ O (NaCl)	I = 0.1	Excitation	248 nm		
File	λ /nm	Time range	Comments	$k(1)/s^{-1}$	error k(1)	A0	A_inf	A_max	A0-Ainf(1)
nal1hcl1	330	6.20E-02	I / 1	6.04E+02	1.71E+01	0.150	0.253	0.273	-0.104
nal1hcl2	330	4.80E-02	I / 2	6.18E+02	1.88E+01	0.084	0.169	0.185	-0.085
nal1hcl3	330	4.80E-02	I / 3	5.94E+02	2.81E+01	0.056	0.116	0.137	-0.060
nal1hcl4	320	4.80E-02	II / 1	6.03E+02	2.68E+01	0.148	0.231	0.264	-0.083
nal1hcl5	320	4.80E-02	II / 2	5.49E+02	3.11E+01	0.048	0.122	0.153	-0.074
nal1hcl6	330	4.80E-02	III / 1	6.10E+02	2.55E+01	0.169	0.273	0.303	-0.104
				5.96E+02	6.93E+00				

o-NBAL in 0.070 M HCl

o-nitrobenzyl alcohol				H ₂ O (NaCl)		Excitation	248 nm		
nal70hcl1	330	8.20E-02	I / 1	3.82E+02	3.99E+00	0.085	0.220	0.232	-0.135
nal70hcl2	330	8.20E-02	I / 2	3.86E+02	7.05E+00	0.088	0.169	0.183	-0.081
nal70hcl3	330	8.20E-02	I / 3	4.50E+02	2.20E+01	0.111	0.147	0.164	-0.036
"	330	8.20E-02	I / 3	3.90E+02	6.92E+00	0.054	0.147	0.164	-0.093
nal70hcl4	310	8.20E-02	II / 1	4.08E+02	7.50E+00	0.111	0.243	0.265	-0.132
nal70hcl5	320	8.00E-02	II / 2	3.97E+02	9.45E+00	0.083	0.180	0.200	-0.097
nal70hcl6	320	8.20E-02	III / 1	3.98E+02	5.80E+00	0.147	0.285	0.303	-0.137
nal70hcl7	320	7.30E-01	III / 1	1.45E+01	1.12E+00	0.287	0.281	0.290	0.006
nal70hcl8	320	6.00E-02	III / 2	3.85E+02	7.15E+00	0.072	0.182	0.201	-0.109
				3.99E+02					

o-NBAL in 0.050 M HCl

o-nitrobenzyl alcohol				H ₂ O (NaCl)		Excitation	248 nm		
nal50hcl1	310	5.10E-02	I / 1	3.24E+02	3.695	0.103	0.266	0.287	
nal50hcl2	325	5.10E-02	I / 2	3.30E+02	5.797	0.102	0.187	0.199	
nal50hcl3	320	5.10E-02	II / 1	3.40E+02	3.308	0.133	0.297	0.316	
nal50hcl4	320	5.10E-02	II / 2	3.21E+02	3.807	0.052	0.198	0.217	
"	320	5.10E-02	II / 2	3.36E+02	5.811	0.096	0.198	0.217	
				3.30E+02					

o-NBAL in 0.030 M HCl

o-nitrobenzyl alcohol				H ₂ O (NaCl)		Excitation	248 nm		
nal30hcl1	320	7.10E-02	I / 1	2.20E+02	2.857	0.149	0.269	0.293	
nal30hcl2	320	7.10E-02	I / 2	2.22E+02	4.078	0.080	0.176	0.202	
nal30hcl3	330	7.10E-02	I / 3	2.20E+02	3.771	0.049	0.125	0.142	
nal30hcl4	310	7.10E-02	II / 1	2.15E+02	3.141	0.106	0.250	0.278	
nal30hcl5	330	7.10E-02	II / 2	2.20E+02	3.225	0.069	0.157	0.175	
nal30hcl6	325	7.10E-02	III / 1	2.24E+02	1.994	0.112	0.248	0.264	

"	325	7.10E-02	III / 1	2.03E+02	1.095	0.020	0.248	0.264
nal30hcl7	325	7.10E-02	III / 2	2.19E+02	3.608	0.090	0.183	0.199

2.20E+02

File	λ/nm	Time range	Comments	$k(1)/\text{s}^{-1}$	error k(1)	A0	A_inf	A_max	A0-Ainf(1)
o-NBAL in 0.020 M HCl		o-nitrobenzyl alcohol		H2O (NaCl)		Excitation		248 nm	
nal20hcl1	320	9.30E-02	I / 1	1.52E+02	1.09	0.139	0.331	0.349	
"	320	9.30E-02	I / 1	1.53E+02	1.409	0.179	0.331	0.349	
nal20hcl2	320	1.20E-01	I / 2	1.57E+02	2.122	0.090	0.186	0.199	
nal20hcl3	310	1.20E-01	II / 1	1.60E+02	1.837	0.108	0.255	0.272	
nal20hcl4	330	1.20E-01	II / 2	1.55E+02	2.057	0.079	0.165	0.180	
nal20hcl5	330	1.20E-01	II / 3	1.48E+02	1.765	0.036	0.134	0.145	
"	330	1.20E-01	II / 3	1.58E+02	3.293	0.076	0.134	0.145	

1.56E+02

o-NBAL in 0.010 M HCl		o-nitrobenzyl alcohol		H2O (NaCl)		Excitation		248 nm 190mJ	
nal10hcl1	410	4.40E-07	I / 1	7.83E+07	2.04E+06	0.029	0.004	0.032	0.025
nal10hcl2	430	4.40E-07	I / 2	6.53E+07	1.61E+06	0.022	0.002	0.025	0.020
nal10hcl3	320	2.00E-01	II / 1	1.15E+02	1.31E+00	0.120	0.270	0.289	-0.150
nal10hcl4	325	2.00E-01	II / 2	1.08E+02	1.66E+00	0.082	0.194	0.211	-0.111
nal10hcl5	330	2.00E-01	III / 1	1.11E+02	1.04E+00	0.113	0.228	0.237	-0.114
nal10hcl6	330	1.30E-01	III / 2	1.06E+02	1.27E+00	0.073	0.182	0.197	-0.108

1.08E+02

o-NBAL in 0.005 M HCl		o-nitrobenzyl alcohol		H2O (NaCl)		Excitation		248 nm 190mJ	
nal5hcl1	410	5.00E-07	I / 1	5.48E+07	4.92E+05	0.050	0.007	0.077	0.043
nal5hcl2	410	5.00E-07	I / 2	5.66E+07	9.19E+05	0.029	0.004	0.051	0.025
nal5hcl3	430	4.90E-07	II / 1	6.19E+07	5.17E+05	0.059	0.007	0.090	0.052
"	430	4.90E-07	II / 1	6.52E+07	9.35E+05	0.037	0.007	0.090	0.031
"	430	4.90E-07	II / 1	5.41E+07	3.55E+05	0.080	0.007	0.090	0.074
nal5hcl4	430	4.90E-07	II / 2	5.40E+07	6.63E+05	0.040	0.004	0.060	0.036

5.85E+07

nal5hcl5	320	1.40E-01	III / 1	8.43E+01	7.05E-01	0.164	0.298	0.311	-0.134
"	320	1.40E-01	III / 1	8.24E+01	4.60E-01	0.101	0.298	0.311	-0.197
nal5hcl6	320	1.40E-01	III / 2	8.41E+01	9.68E-01	0.092	0.213	0.229	-0.121
nal5hcl7	330	1.40E-01	IV / 1	8.66E+01	6.74E-01	0.144	0.257	0.269	-0.113
"	330	1.40E-01	IV / 1	8.13E+01	3.29E-01	0.041	0.257	0.269	-0.217
nal5hcl8	330	1.40E-01	IV / 2	8.53E+01	7.73E-01	0.098	0.205	0.215	-0.107

8.35E+01									
File	λ/nm	Time range	Comments	$k(1)/\text{s}^{-1}$	error $k(1)$	A0	A_inf	A_max	A0-Ainf(1)
o-NBAL in 0.003 M HCl			o-nitrobenzyl alcohol	H2O (NaCl)	I = 0.1	Excitation	248 nm	180mJ	
nal3hcl1	320	2.20E-01	I / 1	6.87E+01	3.44E-01	0.139	0.316	0.325	-0.177
"	320	2.20E-01	I / 1	6.95E+01	6.63E-01	0.222	0.316	0.325	-0.094
nal3hcl2	320	2.20E-01	I / 2	6.81E+01	7.59E-01	0.096	0.208	0.221	-0.112
nal3hcl3	330	2.20E-01	II / 1	6.80E+01	4.29E-01	0.139	0.255	0.264	-0.116
nal3hcl4	330	2.20E-01	II / 2	6.34E+01	3.03E-01	0.050	0.219	0.228	-0.169
"	330	2.20E-01	II / 2	6.59E+01	4.09E-01	0.090	0.219	0.228	
"	330	2.20E-01	II / 2	6.87E+01	8.94E-01	0.156	0.219	0.228	
nal3hcl5	330	2.20E-01	II / 3	6.61E+01	7.79E-01	0.097	0.176	0.185	-0.079
6.67E+01									
nal3hcl6	430	4.90E-07	III / 1	4.57E+07	2.81E+05	0.079	0.007	0.110	
nal3hcl7	430	4.90E-07	III / 2	4.49E+07	4.18E+05	0.048	0.004	0.072	
nal3hcl8	430	4.90E-07	III / 3	4.56E+07	4.88E+05	0.041	0.002	0.056	
nal3hcl9	410	4.90E-07	IV / 1	4.98E+07	6.23E+05	0.042	0.007	0.092	
"	410	4.90E-07	IV / 1	4.45E+07	3.19E+05	0.067	0.007	0.092	
nal3hcl10	410	4.90E-07	IV / 2	4.80E+07	5.48E+05	0.038	0.005	0.063	
4.64E+07									
o-NBAL in 0.002 M HCl			o-nitrobenzyl alcohol	H2O (NaCl)		Excitation	248 nm	180mJ	
nal2hcl1	410	8.30E-07	I / 1	3.35E+07	8.67E+05	0.028	0.006	0.097	
"	410	8.30E-07	I / 1	3.79E+07	2.93E+05	0.088	0.006	0.097	
nal2hcl2	410	7.20E-07	I / 2	3.50E+07	3.78E+05	0.057	0.004	0.071	
nal2hcl3	430	7.20E-07	II / 1	3.79E+07	3.02E+05	0.082	0.005	0.106	
nal2hcl4	430	7.20E-07	II / 2	3.69E+07	4.15E+05	0.054	0.005	0.078	
nal2hcl5	430	7.20E-07	II / 3	3.73E+07	5.19E+05	0.036	0.003	0.051	
3.70E+07									
nal2hcl6	320	2.40E-01	III / 1	5.91E+01	3.67E-01	0.175	0.295	0.305	
nal2hcl7	320	2.40E-01	III / 2	5.98E+01	5.48E-01	0.136	0.229	0.240	
"	320	2.40E-01	III / 2	5.63E+01	2.75E-01	0.058	0.229	0.240	
nal2hcl8	330	2.40E-01	IV / 1	5.80E+01	3.00E-01	0.146	0.250	0.256	
nal2hcl9	330	2.40E-01	IV / 2	5.80E+01	3.59E-01	0.088	0.185	0.192	
5.74E+01									
o-NBAL in 0.001 M HCl			o-nitrobenzyl alcohol	H2O (NaCl)		Excitation	248 nm	190mJ	
nal1hcl1	330	2.80E-01	I / 1	4.24E+01	2.70E-01	0.133	0.251	0.261	

nal1hcl2	330	2.80E-01	I / 2	4.18E+01	3.01E-01	0.103	0.209	0.219
nal1hcl3	320	3.70E-01	II / 1	4.44E+01	2.24E-01	0.121	0.301	0.311
nal1hcl4	320	3.70E-01	II / 2	4.44E+01	4.41E-01	0.116	0.241	0.255
				4.33E+01				
nal1hcl5	430	1.00E-06	III / 1	2.40E+07	1.34E+05	0.109	0.009	0.115
nal1hcl6	430	1.00E-06	III / 2	2.45E+07	2.22E+05	0.067	0.007	0.073
nal1hcl7	410	8.60E-07	IV / 1	2.70E+07	1.49E+05	0.103	0.006	0.114
nal1hcl8	410	8.60E-07	IV / 2 210mJ	2.63E+07	1.99E+05	0.073	0.004	0.085

2.59E+07

File	λ /nm	Time range	Comments	$k(1)/s^{-1}$	error k(1)	A0	A_inf	A_max	A0-Ainf(1)
o-NBAL in 0.001 M HCl			o-nitrobenzyl alcohol	H2O		Excitation		248 nm	
nal1mMhcl1	410	1.50E-06	I / 1	2.56E+07	2.52E+05	0.104	0.008	0.112	0.096
nal1mMhcl2	410	7.30E-07	I / 1	2.65E+07	2.38E+05	0.089	0.008	0.112	0.081
nal1mMhcl3	410	7.30E-07	I / 2	2.80E+07	3.81E+05	0.060	0.005	0.075	0.055
nal1mMhcl4	410	7.30E-07	I / 3	2.50E+07	5.09E+05	0.039	0.004	0.056	0.035
nal1mMhcl5	410	7.30E-07	I / 4	2.59E+07	7.30E+05	0.032	0.005	0.042	0.027
nal1mMhcl6	410	7.30E-07	I / 5	3.13E+07	9.19E+05	0.030	0.004	0.037	0.026
				2.62E+07					
nal1mMhcl7	320	7.30E-07	II / 1	1.43E+07	1.24E+06	0.071	0.100	0.128	-0.029
nal1mMhcl8	330	7.30E-07	II / 2	1.22E+07	1.42E+07	0.011	0.059	0.084	-0.048
nal1mMhcl9	330	3.90E-01	II / 3	4.16E+01	3.67E-01	0.064	0.124	0.130	-0.060
nal1mMhcl10	320	4.00E-01	II / 4	4.62E+01	2.87E+00	0.030	0.062	0.078	-0.031
				4.30E+01					
nal1mMhcl11	320	4.00E-01	III / 1	4.33E+01	3.53E-01	0.054	0.176	0.192	-0.122
nal1mMhcl12	320	4.00E-01	III / 2	4.11E+01	5.70E-01	0.043	0.124	0.136	-0.081
nal1mMhcl14	410	1.60E-06	III / 4	2.62E+07	1.60E+06	0.017	0.003	0.022	0.015

o-NBAL in 0.42 mM HCl

				H2O		Excitation		248 nm	
nal04mMhcl1	410	2.30E-06	I / 1	1.91E+07	2.84E+05	0.071	0.009	0.081	0.062
nal04mMhcl2	410	8.20E-07	I / 1	1.90E+07	2.50E+05	0.058	0.009	0.081	0.049
nal04mMhcl3	410	8.20E-07	I / 2	2.03E+07	3.64E+05	0.040	0.005	0.051	0.035
nal04mMhcl4	410	8.20E-07	I / 3	1.92E+07	4.73E+05	0.032	0.005	0.043	0.026
nal04mMhcl5	410	8.20E-07	I / 4	1.91E+07	6.38E+05	0.023	0.004	0.031	0.018
				1.92E+07	5.46E+05				
nal04mMhcl6	310	1.20E-06	II / 1	1.39E+07	2.23E+06	0.082	0.094	0.114	-0.012
nal04mMhcl7	330	1.20E-06	II / 2	5.12E+06	1.10E+06	0.045	0.051	0.067	-0.006
"	330	1.20E-06	II / 2	8.37E+06	1.76E+06	0.045	0.051	0.067	-0.006

nal04mMhcl8									
nal04mMhcl9	330	4.30E-01	II / 1	3.48E+01	2.65E-01	0.050	0.119	0.125	-0.069
nal04mMhcl10	330	4.30E-01	II / 2	3.44E+01	3.90E-01	0.039	0.079	0.086	-0.040
nal04mMhcl11	330	4.30E-01	II / 3	3.16E+01	6.91E-01	0.026	0.051	0.055	-0.025
				3.40E+01	1.58E+00				
nal04mMhcl12	310	4.30E-01	III / 2	3.50E+01	4.64E-01	0.031	0.094	0.104	-0.063
nal04mMhcl13	400	4.30E-06	III / 3	1.76E+07	2.28E+06	0.011	0.003	0.013	0.009
nal04mMhcl14	400	7.50E-06	IV / 1	1.86E+07	2.31E+05	0.056	0.009	0.071	0.047
nal04mMhcl15	400	7.50E-06	IV / 2	1.90E+07	3.59E+05	0.038	0.006	0.047	0.033

o-NBAL in 0.1 M NaOH

o-nitrobenzyl alcohol				H2O (NaCl)		Excitation		248 nm					
File	λ /nm	Time range	Comments	$k(1)/s^{-1}$	error k(1)	A0	A_inf	A_max	A0-Ainf(1)	k(2)	error k(2)	<u>A0-Ainf(2)</u>	A2/A1
nal100oh1	320	2.00E-06	180mJ I / 1	1.03E+07	6.50E+05	0.303	0.342	0.367	-0.039				
nal100oh2	320	2.00E-06	I / 2	8.57E+06	5.10E+05	0.281	0.320	0.349	-0.039				
nal100oh3	330	2.00E-06	I / 3	1.75E+07	1.75E+06	0.215	0.238	0.257	-0.022				
				1.21E+07									
nal100oh4	390	1.70E-06	II / 1	8.05E+06	2.15E+05	0.056	0.043	0.064	0.014				
nal100oh5	410	2.10E-06	II / 2	1.00E+07	1.20E+05	0.060	0.028	0.067	0.032				
nal100oh6	430	2.10E-06	II / 3	8.10E+06	1.74E+05	0.033	0.018	0.066	0.015				
"	430	2.10E-06	II / 3	6.28E+06	4.31E+05	0.063	0.018	0.066	0.017	1.92E+07	1.24E+06	2.82E-02	1.6861
				1.03E+07									
nal100oh7	500	2.10E-06	III / 1	1.03E+07	2.00E+05	0.026	0.006	0.117	0.020				
"	500	2.10E-06	III / 1	8.58E+06	3.57E+05	0.111	0.006	0.117	0.029	3.11E+07	8.74E+05	7.60E-02	2.6153
nal100oh8	470	2.10E-06	III / 2	1.35E+07	8.15E+04	0.094	0.010	0.107	0.084				
"	470	2.10E-06	III / 2	7.40E+06	2.86E+05	0.100	0.010	0.107	0.032	2.29E+07	7.77E+05	5.86E-02	1.8409
nal100oh9	430	2.10E-06	III / 3	7.50E+06	1.76E+05	0.032	0.019	0.071	0.013				
"	430	2.10E-06	III / 3	1.17E+07	1.12E+05	0.063	0.019	0.071					
"	430	2.10E-06	III / 3	4.74E+06	3.44E+05	0.066	0.019	0.071	0.011	1.81E+07	6.80E+05	3.64E-02	3.1972
				7.42E+06						2.44E+07			

o-NBAL in 0.05 M NaOH

o-nitrobenzyl alcohol				H2O (NaCl)		Excitation		248 nm					
nal50oh1	390	1.90E-06	I / 1	7.89E+06	2.32E+05	0.054	0.042	0.067	0.012				
"	390	1.90E-06	I / 1	8.24E+06	1.95E+05	0.057	0.042	0.067	0.016				
nal50oh2	390	1.90E-06	I / 2	7.27E+06	2.26E+05	0.051	0.039	0.058	0.012				
nal50oh3	410	1.90E-06	I / 3	9.81E+06	1.77E+05	0.047	0.025	0.055	0.022				
nal50oh4	410	1.90E-06	II / 1	1.02E+07	1.50E+05	0.058	0.030	0.084	0.027				

"	410	1.90E-06	II / 1	3.69E+06	4.77E+05	0.082	0.030	0.084	0.007096	1.53E+07	4.64E+05	4.45E-02	6.2774
nal50oh5	430	1.90E-06	II / 2	8.44E+06	2.40E+05	0.027	0.016	0.070	0.011				
"	430	1.90E-06	II / 2	1.28E+07	1.10E+05	0.064	0.016	0.070	0.048				
"	430	1.90E-06	II / 2	3.94E+06	4.04E+05	0.066	0.016	0.070	0.007201	1.67E+07	4.50E+05	4.31E-02	5.9827
nal50oh6	470	1.90E-06	II / 3	1.34E+07	8.42E+04	0.083	0.012	0.092	0.071				
"	470	1.90E-06	II / 3	6.84E+06	4.32E+05	0.087	0.012	0.092	0.021126	1.96E+07	7.41E+05	5.41E-02	2.5629
				1.21E+07									
nal50oh7	310	1.30E-06	III / 1	6.72E+06	5.24E+05	0.263	0.297	0.330	-0.034				
nal50oh8	320	2.00E-06	III / 2	9.28E+06	6.52E+05	0.300	0.338	0.367	-0.038				
nal50oh9	330	2.00E-06	III / 3	1.24E+07	1.36E+06	0.236	0.255	0.276	-0.019				

1.09E+07

File	λ /nm	Time range	Comments	$k(1)/s^{-1}$	error k(1)	A0	A_inf	A_max	A0-Ainf(1)	k(2)	error k(2)	<u>A0-Ainf(2)</u>	A2/A1
o-NBAL in 0.03 M NaOH				o-nitrobenzyl alcohol		H2O (NaCl)		Excitation		248 nm			
nal30oh1	500	1.60E-06	I / 1	1.12E+07	1.88E+05	0.028	0.006	0.113	0.022				
"	500	1.60E-06	I / 1	9.72E+06	3.77E+05	0.082	0.006	0.113	0.030	3.49E+07	1.51E+06	4.60E-02	1.5512
nal30oh2	470	1.60E-06	I / 2	1.53E+07	8.35E+04	0.092	0.009	0.110	0.083				
"	470	1.60E-06	I / 2	8.38E+06	4.03E+05	0.096	0.008	0.110	0.028	2.34E+07	8.14E+05	5.96E-02	2.0965
nal30oh3	430	1.60E-06	I / 3	1.11E+07	2.00E+05	0.035	0.015	0.066					
"	430	1.60E-06	I / 3	4.30E+06	6.64E+05	0.061	0.015	0.066	0.006	1.65E+07	5.41E+05	3.96E-02	6.7759
nal30oh4	390	1.60E-06	II / 1	1.10E+07	2.13E+05	0.055	0.037	0.060					
nal30oh5	400	1.60E-06	II / 2	9.83E+06	2.37E+05	0.041	0.027	0.053					
nal30oh6	430	1.60E-06	II / 3	1.00E+07	1.65E+05	0.034	0.016	0.065					
"	430	1.60E-06	II / 3	6.62E+06	4.73E+05	0.060	0.015	0.065	0.014	2.11E+07	1.06E+06	3.07E-02	2.2158
				8.24E+06						2.65E+07			
				1.21E+07									
nal30oh7	320	1.40E-06	III / 1	9.44E+06	4.02E+05	0.240	0.280	0.299					
nal30oh8	325	1.40E-06	III / 2	9.24E+06	5.74E+05	0.285	0.313	0.336					
nal30oh9	335	5.20E-07	III / 3	2.48E+07	2.14E+06	0.191	0.206	0.220					
nal30oh10	310	1.00E-06	IV / 1	6.81E+06	5.71E+05	0.277	0.309	0.348					
nal30oh11	320	3.60E-04	IV / 2	6.42E+03	5.58E+01	0.339	0.250	0.347					
nal30oh12	320	3.70E-06	IV / 2	6.54E+06	1.47E+06	0.315	0.343	0.370					
nal30oh13	430	1.90E-06	IV / 5	8.08E+06	2.57E+05	0.025	0.015	0.040					
				1.14E+07									

o-NBAL in 0.02 M NaOH

o-nitrobenzyl alcohol				H2O (NaCl)		Excitation		248 nm					
nal20oh1	335	6.10E-07	I / 1	2.28E+07	9.77E+05	0.189	0.215	0.225	-0.025				
"	335	6.10E-07	I / 1	1.68E+07	1.04E+06	0.199	0.215	0.225	-0.016				

nal10oh8	330	1.80E-06	II / 4	1.24E+07	4.42E+05	0.093	0.128	0.139
nal10oh9	320	1.10E-06	III / 1	9.30E+06	4.43E+05	0.318	0.359	0.383
nal10oh10	330	1.10E-06	III / 2	1.49E+07	6.62E+05	0.199	0.230	0.246
nal10oh11	335	1.00E-06	III / 3	1.96E+07	1.39E+06	0.147	0.165	0.180
nal10oh12	335	9.10E-05	IV / 1	1.56E+04	1.74E+02	0.214	0.158	0.216
nal10oh13	335	1.00E-06	IV / 1	1.83E+07	1.52E+06	0.190	0.214	0.222
nal10oh14	335	2.10E-06	IV / 2	1.20E+07	2.30E+06	0.171	0.188	0.200
nal10oh15	335	3.50E-04	IV / 2	1.38E+04	6.19E+01	0.187	0.142	0.190
nal10oh16	335	3.50E-04	IV / 3	1.52E+04	8.71E+01	0.174	0.138	0.177
				1.34E+07				

p[H⁺] = 3.56

[MeCOOH]/[NaOH] =

11.0

o-nitrobenzyl alcohol

o-NBAL in 50 mM acetate buffer

I=0.1

[Buffer]= 50 mM

Excitation 248 nm

File	λ /nm	Time range	Comments	$k(1)/s^{-1}$	error k(1)	A0	A_inf	A_max	A0-Ainf(1)	$k(2)/s^{-1}$	error k(2)	A0-Ainf(2)	A2/A1
nal05ac1	410	7.50E-06 I / 1		1.93E+07	5.60E+05	0.075	0.008	0.107	0.067				
nal05ac2	410	1.30E-06 I / 1		2.25E+07	5.28E+05	0.100	0.010	0.107	0.090				
nal05ac3	410	9.30E-07 I / 2		2.17E+07	3.06E+05	0.061	0.007	0.073	0.054				
nal05ac4	410	9.30E-07 I / 3		2.08E+07	3.76E+05	0.041	0.005	0.055	0.036				
nal05ac5	430	9.30E-07 I / 4		2.10E+07	6.27E+05	0.026	0.005	0.044	0.021				
				2.12E+07									
nal05ac6	330	1.80E-03 II / 1		1.36E+02	2.48E+01	0.056	0.242	0.097	-0.185				
nal05ac7	330	1.00E-01 II / 2		1.08E+02	7.48E-01	0.052	0.127	0.134	-0.074				
nal05ac8	330	2.00E-01 II / 3		1.07E+02	2.22E+00	0.047	0.092	0.105	-0.045				
nal05ac9	330	2.00E-01 II / 4		1.03E+02	1.76E+00	0.045	0.075	0.080	-0.030				
				1.13E+02									

o-NBAL in 40 mM acet.buffer

I=0.1

[Buffer]= 40 mM

o-nitrobenzyl alcohol

nal04ac1	410	7.00E-07 I / 1		1.87E+07	1.95E+05	0.054	0.009	0.131	0.045				
nal04ac2	410	7.00E-07 I / 2		1.87E+07	2.52E+05	0.042	0.006	0.093	0.036				
nal04ac3	410	7.00E-07 I / 3		2.07E+07	2.81E+05	0.042	0.005	0.069	0.037				
				1.94E+07									
nal04ac6	320	1.80E-01 II / 1		8.97E+01	6.17E-01	0.140	0.238	0.245	-0.098				
"	320	1.80E-01 II / 1		8.75E+01	9.74E-01	0.073	0.238	0.245	-0.165	4.32E+02	4.63E+01	-0.0291	0.1761
nal04ac7	320	1.80E-01 II / 2		8.44E+01	2.77E+00	0.113	0.154	0.166	-0.041				
"	320	3.50E-01 II / 2		9.17E+01	1.52E+00	0.071	0.154	0.166	-0.083				
nal04ac9	330	3.50E-01 II / 4		8.90E+01	2.967	0.057	0.081	0.087	-0.024				
nal04ac10	330	3.50E-01 II / 5		8.63E+01	3.685	0.048	0.068	0.074	-0.020				
				8.74E+01									

o-NBAL in 35mM acet.buffer

I=0.1

[Buffer]= 35 mM

o-nitrobenzyl alcohol

nal035ac1	410	2.10E-06 I / 1		1.98E+07	1.63E+05	0.097	0.010	0.122	0.087				
"	410	2.10E-06 I / 1		1.66E+07	3.22E+05	0.043	0.010	0.122	0.033				
"	410	2.10E-06 I / 1		7.00E+06	1.34E+06	0.099	0.010	0.122	0.089	2.34E+07	8.04E+05	0.0800	
nal035ac2	410	1.10E-06 I / 2		1.52E+07	4.52E+05	0.024	0.008	0.094	0.016				
"	410	1.10E-06 I / 2		1.96E+07	1.41E+05	0.083	0.008	0.094	0.075				
nal035ac3	410	1.10E-06 I / 3		1.88E+07	3.53E+05	0.033	0.005	0.057	0.028				

nal035ac4	450	1.10E-06 I / 4	2.21E+07	5.11E+05	0.025	0.003	0.044	0.022
nal035ac5	320	1.10E-06 I / 5	1.75E+07	1.86E+06	0.105	0.123	0.146	-0.018
			1.70E+07					
nal035ac10	320	3.50E-01 III/1	7.99E+01	1.57E+00	0.152	0.196	0.203	-0.044
"	320	3.50E-01 III/1	8.66E+01	7.19E-01	0.088	0.196	0.203	-0.108
nal035ac11	320	2.70E-01 III/ 2	8.80E+01	1.42E+00	0.065	0.127	0.139	-0.062
nal035ac12	320	2.70E-01 III/ 3	8.53E+01	2.43E+00	0.049	0.088	0.098	-0.039
			8.49E+01					

o-NBAL in 25mM acet.buffer

I=0.1 [Buffer]= 25mM

o-nitrobenzyl alcohol

nal025ac1	410	1.00E-06 I / 1	1.69E+07	1.70E+05	0.051	0.010	0.141	0.041			
"	410	1.00E-06 I / 1	1.83E+07	7.11E+04	0.128	0.010	0.141	0.118			
"	410	1.00E-06 I / 1	1.51E+07	8.13E+05	0.123	0.010	0.141	0.074	2.94E+07	4.00E+06	0.0390
nal025ac2	410	1.00E-06 I / 2	1.55E+07	2.34E+05	0.032	0.006	0.097	0.027			
"	410	1.00E-06 I / 2	1.81E+07	1.04E+05	0.083	0.006	0.097	0.077			
"	410	1.00E-06 I / 2	9.14E+06	1.04E+06	0.080	0.006	0.097	0.017	2.35E+07	1.07E+06	0.0573
nal025ac3	410	1.00E-06 I / 3	1.49E+07	2.79E+05	0.024	0.004	0.074	0.020			
"	410	1.00E-06 I / 3	1.84E+07	1.32E+05	0.063	0.005	0.074	0.059			
"	410	1.00E-06 I / 3	1.16E+07	1.16E+06	0.061	0.004	0.074	0.022	2.75E+07	2.46E+06	0.0343
nal025ac4	450	1.00E-06 I / 4	1.65E+07	4.37E+05	0.018	0.002	0.056	0.016			
			1.39E+07						2.68E+07		
nal025ac6	320	2.50E-06 II / 1	2.65E+07	1.54E+07	0.112	0.120	0.140	-0.008			
nal025ac7	320	7.30E-05 II / 1	7.65E+04	1.21E+03	0.115	0.092	0.123	0.024			
nal025ac9	330	1.70E-04 II / 3	2.73E+04	3.02E+03	0.052	0.045	0.066	0.006			
nal025ac10	330	1.10E-01 II / 5	7.21E+01	1.32E+00	0.042	0.070	0.077	-0.029			
			7.31E+01								
nal025ac11	320	2.60E-01 III / 1	6.81E+01	7.14E-01	0.154	0.219	0.227	-0.065			
"	320	2.60E-01 III / 1	7.51E+01	4.07E-01	0.083	0.219	0.227	-0.136			
nal025ac12	320	2.60E-01 III / 2	7.26E+01	1.51E+00	0.059	0.091	0.098	-0.031			
"	320	2.60E-01 III / 2	7.60E+01	1.08E+00	0.044	0.091	0.098	-0.047			
nal025ac13	320	2.60E-01 III / 3	7.47E+01	2.56E+00	0.036	0.059	0.069	-0.022			
nal025ac14	330	2.60E-01 III / 4	7.03E+01	1.08E+00	0.040	0.070	0.075	-0.030			
nal025ac15	330	2.60E-01 III / 5	7.61E+01	2.01E+00	0.033	0.054	0.060	-0.021			

o-NBAL in 17.5mM acet.buffer

I=0.1 [Buffer]= 17.5 mM

o-nitrobenzyl alcohol

nal0175ac1	410	9.20E-07 I / 1	1.29E+07	5.30E+05	1.21E-01	9.61E-03	1.34E-01	0.0641	2.99E+07	2.30E+06	0.0472	0.7372
------------	-----	----------------	----------	----------	----------	----------	----------	--------	----------	----------	--------	--------

"	410	9.20E-07 I / 1	1.68E+07	8.53E+04	1.02E-01	9.96E-03	1.34E-01						
nal0175ac2	410	9.20E-07 I / 2	1.28E+07	2.05E+06	9.41E-02	6.31E-03	9.86E-02	0.0366	2.20E+07	3.07E+06	0.0511	1.3966	
"	410	9.20E-07 I / 2	1.71E+07	9.27E+04	8.70E-02	6.46E-03	9.86E-02						
nal0175ac3	410	9.20E-07 I / 3	1.25E+07	1.10E+06	7.55E-02	5.22E-03	8.04E-02	0.0368	2.58E+07	3.23E+06	0.0335	0.9081	
"	410	9.20E-07 I / 3	1.65E+07	1.14E+05	6.53E-02	5.42E-03	8.04E-02						
			1.27E+07						2.59E+07				
nal0175ac6	320	1.30E-06 II / 1	1.51E+07	2.50E+06	1.18E-01	1.27E-01	1.42E-01						
nal0175ac7	320	1.70E-05 II / 1	8.32E+04	5.55E+03	1.27E-01	9.99E-02	1.34E-01						
nal0175ac8	320	2.90E-04 II / 2	5.68E+04	3.07E+03	8.10E-02	6.49E-02	9.07E-02						
nal0175ac9	320	1.50E-03 II / 3	-1.72E+06	2.72E+02	3.25E-02	1.27E-02	4.70E-02						
nal0175ac10	320	1.50E-01 II / 4	7.19E+01	9.31E-01	3.63E-02	7.31E-02	7.91E-02						
nal0175ac11	330	1.50E-01 II / 5	5.71E+01	8.08E-01	4.43E-02	6.93E-02	7.42E-02						
			5.96E+01										
nal0175ac13	320	2.50E-01 III / 1	6.04E+01	5.32E-01	1.46E-01	2.13E-01	2.21E-01						
"	320	2.50E-01 III / 1	5.28E+01	2.34E+00	6.44E-02	2.13E-01	2.21E-01	-0.0938	1.15E+02	1.19E+01	-0.0553		
nal0175ac14	320	2.50E-01 III / 2	6.18E+01	9.76E-01	9.46E-02	1.33E-01	1.39E-01						
nal0175ac15	320	2.50E-01 III / 3	6.30E+01	8.29E-01	4.29E-02	9.38E-02	1.02E-01						
nal0175ac16	330	2.50E-01 III / 4	6.27E+01	9.05E-01	4.46E-02	8.43E-02	9.17E-02						
o-NBAL in 12.5mM acet.buffer				I=0.1	[Buffer]=	12.5 mJ			o-nitrobenzyl alcohol				
nal0125ac1	320	3.50E-01 I / 1	5.67E+01	4.71E-01	1.39E-01	2.15E-01	2.24E-01						
"	320	3.50E-01 I / 1	5.40E+01	1.33E+00	6.32E-02	2.15E-01	2.24E-01	-0.1221	1.43E+02	2.20E+01	-0.0302		
nal0125ac2	320	3.50E-01 I / 2	5.33E+01	7.11E-01	9.56E-02	1.38E-01	1.44E-01						
"	320	3.50E-01 I / 2	5.31E+01	1.14E+00	4.71E-02	1.38E-01	1.44E-01	-0.0791	1.76E+02	5.21E+01	-0.0118		
nal0125ac3	320	3.50E-01 I / 3	5.67E+01	1.07E+00	5.79E-02	9.53E-02	1.02E-01						
nal0125ac4	330	3.50E-01 I / 4	5.59E+01	8.48E-01	4.57E-02	7.93E-02	8.45E-02						
			5.44E+01										
nal0125ac5	410	8.30E-07 II / 1	1.32E+07	7.69E+05	1.13E-01	8.42E-03	1.25E-01	0.0771	2.99E+07	6.78E+06	0.0272		
"	410	8.30E-07 II / 1	1.58E+07	1.08E+05	1.15E-01	8.76E-03	1.25E-01						
nal0125ac6	410	8.30E-07 II / 2	1.17E+07	1.61E+06	7.92E-02	6.29E-03	8.89E-02	0.0404	2.55E+07	5.46E+06	0.0326		
"	410	8.30E-07 II / 2	1.56E+07	1.62E+05	7.97E-02	6.63E-03	8.90E-02						
			1.25E+07						2.77E+07				
o-NBAL in 10 mM acet.buffer				I=0.1	[Buffer]=	10 mM			200mJ 0.5/5	o-nitrobenzyl alcohol			
nal01ac1	410	1.60E-06 I / 1	1.48E+07	1.37E+05	0.109	0.009	0.125						
"	410	1.60E-06 I / 1	1.04E+07	8.27E+05	0.113	0.009	0.125	0.053	2.55E+07	3.07E+06	0.0509		

nal01ac2	410	1.50E-06 I / 2	1.32E+07	1.35E+05	0.053	0.006	0.085				
"	410	1.50E-06 I / 2	1.03E+07	6.71E+05	0.074	0.006	0.084	0.037	2.58E+07	2.95E+06	0.0309
nal01ac3	410	1.10E-06 I / 3	1.48E+07	1.25E+05	0.054	0.005	0.063				
			1.04E+07						2.56E+07		
nal01ac5	320	1.60E-01 II / 1	4.78E+01	3.27E-01	0.124	0.198	0.207				
"	320	1.60E-01 II / 1	4.54E+01	8.63E-01	0.055	0.198	0.207	-0.1139	1.35E+02	1.40E+01	-0.0293
nal01ac6	320	7.00E-03 II / 1	1.29E+02	0.00E+00	0.052	0.132	0.113	-0.0903	2.93E+03	8.25E+02	0.0103
nal01ac7	320	1.80E-01 II / 2	5.30E+01	8.32E-01	0.043	0.095	0.105				
nal01ac8	330	1.80E-01 II / 3	5.06E+01	9.30E-01	0.043	0.077	0.087				
			5.05E+01								

o-NBAL in 5 mM acet.buffer

I=0.1

[Buffer]= 5 mM

190mJ 0.5/5

o-nitrobenzyl alcohol

nal005ac1	330	3.30E-01 I / 1	3.61E+01	2.36E-01	0.161	0.228	0.234				
"	330	3.30E-01 I / 1	3.60E+01	0.00E+00	0.073	0.228	0.234				
"	330	3.30E-01 I / 1	4.10E+01	4.70E-01	0.083	0.229	0.234	-0.139	8.5193	2.549	-0.0071
nal005ac2	330	7.20E-01 I / 2	3.39E+01	4.21E-01	0.111	0.158	0.165				
"	330	7.20E-01 I / 2	3.72E+01	2.94E-01	0.073	0.157	0.165				
nal005ac3	330	3.80E-01 I / 3	3.67E+01	3.89E-01	0.046	0.112	0.119				
			3.57E+01								
nal005ac4	410	1.50E-06 II / 1	8.78E+06	2.34E+05	0.099	0.010	0.112	0.055203	3.04E+07	2.26E+06	0.0334
"	410	1.50E-06 II / 1	1.17E+07	8.07E+04	0.091	0.010	0.112				
nal005ac7	430	1.50E-06 III / 1	9.40E+06	2.00E+05	0.096	0.008	0.101	0.063	3.36E+07	3.12E+06	0.0245
nal005ac8	430	1.50E-06 III / 2	9.65E+06	2.93E+05	0.079	0.006	0.084	0.051	3.13E+07	3.50E+06	0.0224
			9.52E+06						3.24E+07		

p[H⁺] = 4.16

[MeCOOH]/[NaOH] =

3.52

o-NBAL in 50 mM acetate buffer

I=0.1

[Buffer]= 50 mM

180-200mJ

o-nitrobenzyl alcohol

File	λ /nm	Time range	Comments	$k(1)/s^{-1}$	error k(1)	A0	A_inf	A_max	A0-Ainf(1)	$k(2)/s^{-1}$	error k(2)	A0-Ainf(2)	A2/A1
nal50ace1	470	1.10E-06 I / 1		1.50E+07	2.53E+05	0.033	0.003	0.090	0.030				
"	470	1.10E-06 I / 1		6.86E+06	2.38E+06	0.087	0.003	0.090	0.007487	1.88E+07	7.77E+05	0.0767	
nal50ace2	450	1.10E-06 I / 2		1.52E+07	3.05E+05	0.027	0.004	0.093	0.023				
"	450	1.10E-06 I / 2		1.68E+07	1.02E+05	0.083	0.004	0.093	0.079				
nal50ace3	430	1.10E-06 I / 3		1.60E+07	2.87E+05	0.029	0.004	0.079	0.025				
"	430	1.10E-06 I / 3		1.70E+07	1.23E+05	0.068	0.004	0.079	0.064				
nal50ace4	430	1.10E-06 II / 1		1.48E+07	1.61E+05	0.051	0.005	0.134	0.045				

"	430	1.10E-06 II / 1	1.70E+07	8.52E+04	0.114	0.006	0.134	0.109			
"	430	1.10E-06 II / 1	1.34E+07	1.02E+06	0.121	0.005	0.134	6.60E-02	2.56E+07	3.38E+06	0.0495
nal50ace5	410	9.30E-07 II / 2	1.65E+07	1.05E+05	0.075	0.005	0.096	0.070			
nal50ace6	410	9.30E-07 II / 3	1.66E+07	1.65E+05	0.049	0.004	0.066	0.045			
			1.61E+07								
nal50ace7	320	7.30E-07 III / 1	1.86E+02	6.27E+00	0.172	0.227	0.247	-0.055			
nal50ace8	325	7.30E-07 III / 2	1.97E+02	5.31E+00	0.139	0.189	0.206	-0.050			
"	325	7.30E-07 III / 2	1.95E+02	5.07E+00	0.066	0.189	0.206	-0.094	1.29E+03	2.49E+02	-0.0292
nal50ace9	330	7.30E-07 IV / 1	1.91E+02	2.92E+00	0.138	0.208	0.222	-0.071			
"	330	7.30E-07 IV / 1	1.87E+02	4.05E+00	0.067	0.208	0.222	-0.101	1.09E+03	1.23E+02	-0.0405
nal50ace10	330	7.30E-07 IV / 2	2.02E+02	4.49E+00	0.090	0.143	0.160	-0.053			
"	330	7.30E-07 IV / 2	2.00E+02	5.57E+00	0.057	0.143	0.160	-0.070	1.58E+03	4.77E+02	-0.0166
			1.92E+02						1.32E+03		

o-NBAL in 35 mM acetate buffer			I=0.1	[Buffer]=	35 mM	H2O	o-nitrobenzyl alcohol				
nal35ace1	330	1.00E-01 I / 1	1.50E+02	3.49E+00	0.144	0.202	0.219	-0.057			
"	330	1.00E-01 I / 1	1.46E+02	3.87E+00	0.062	0.202	0.219	-0.104	7.91E+02	1.31E+02	-0.0353
nal35ace2	330	1.00E-01 I / 2	1.49E+02	3.43E+00	0.106	0.151	0.161	-0.045			
"	330	1.00E-01 I / 2	1.46E+02	3.51E+00	0.048	0.151	0.161	-0.075	1.04E+03	1.61E+02	-0.0275
nal35ace3	330	1.00E-01 I / 3	1.45E+02	5.71E+00	0.075	0.107	0.125	-0.032			
nal35ace4	320	1.00E-01 II / 1	1.47E+02	3.02E+00	0.174	0.240	0.256	-0.066			
"	320	1.00E-01 II / 1	1.42E+02	4.27E+00	0.088	0.240	0.256	-0.10990	6.38E+02	9.70E+01	-0.0419
nal35ace5	320	1.00E-01 II / 2	1.38E+02	1.07E+01	0.076	0.192	0.221	-0.078	5.32E+02	1.48E+02	-0.0380
			1.43E+02						7.49E+02		
nal35ace6	410	1.10E-06 III / 2	1.43E+07	1.14E+05	0.070	0.004	0.082	0.066			
"	410	1.10E-06 III / 2	1.38E+07	1.81E+05	0.044	0.004	0.082	0.039			
nal35ace7	420	1.10E-06 III / 3	1.38E+07	1.17E+05	0.055	0.004	0.070	0.051			
"	420	1.10E-06 III / 3	1.33E+07	2.25E+05	0.030	0.004	0.070	0.026			
nal35ace8	430	1.10E-06 IV / 1	1.39E+07	5.64E+04	0.128	0.006	0.139	0.122			
"	430	1.10E-06 IV / 1	1.08E+07	9.58E+05	0.130	0.006	0.139	0.06420	1.96E+07	2.28E+06	0.0601
nal35ace9	440	1.10E-06 IV / 2	1.30E+07	1.46E+05	0.046	0.004	0.106	0.042			
"	440	1.10E-06 IV / 2	1.21E+07	9.42E+05	0.098	0.004	0.106	0.06309	2.32E+07	4.68E+06	0.0309
nal35ace10	450	1.10E-06 IV / 3	1.45E+07	1.11E+05	0.060	0.003	0.067	0.058			
"	450	1.10E-06 IV / 3	7.73E+06	2.54E+06	0.061	0.003	0.067	0.00945	1.67E+07	1.31E+06	0.0492
			1.02E+07						1.99E+07		

1.37E+07

o-NBAL in 25 mM acetate buffer				I=0.1	[Buffer]= 25 mM		H2O	o-nitrobenzyl alcohol			
nal25ace1	410	1.20E-06 I / 1	1.09E+07	1.15E+05	0.055	0.007	0.126	0.048			
"	410	1.20E-06 I / 1	1.01E+07	3.01E+05	0.122	0.007	0.126	0.084055	2.70E+07	3.21E+06	0.0305
nal25ace2	430	1.20E-06 I / 2	1.08E+07	8.72E+04	0.065	0.005	0.110	0.060			
"	430	1.20E-06 I / 2	1.02E+07	2.86E+05	0.108	0.005	0.110	0.08138	2.75E+07	4.27E+06	0.0223
nal25ace3	450	1.20E-06 I / 3	1.13E+07	1.50E+05	0.039	0.003	0.075	0.036			
"	450	1.20E-06 I / 3	1.13E+07	2.12E+05	0.066	0.003	0.075	0.05452	5.85E+07	1.47E+07	0.0083
nal25ace4	490	1.20E-06 II / 1	1.39E+07	1.70E+05	0.050	0.002	0.059	0.048			
"	490	1.20E-06 II / 1	1.08E+07	5.63E+05	0.054	0.002	0.059	0.03492	3.48E+07	6.64E+06	0.0168
nal25ace5	430	1.20E-06 II / 2	1.20E+07	7.32E+04	0.088	0.005	0.103	0.084			
"	430	1.20E-06 II / 2	1.09E+07	2.45E+05	0.092	0.004	0.103	0.07308	3.71E+07	6.85E+06	0.0146
nal25ace6	430	1.20E-06 II / 3	1.12E+07	1.08E+05	0.051	0.003	0.078	0.048			
				1.06E+07					3.95E+07		
nal25ace7	320	1.30E-01 III / 1	1.15E+02	2.74E+00	0.156	0.240	0.267	-0.084			
"	320	1.30E-01 III / 1	1.09E+02	4.32E+00	0.084	0.240	0.267	-0.11389	5.36E+02	1.15E+02	-0.0416
nal25ace8	325	1.30E-01 III / 2	1.11E+02	3.84E+00	0.117	0.177	0.211	-0.060			
"	325	1.30E-01 III / 2	1.02E+02	6.26E+00	0.059	0.177	0.210	-0.07971	4.63E+02	1.17E+02	-0.0381
nal25ace9	332	1.30E-01 III / 3	1.33E+02	3.16E+00	0.065	0.121	0.127	-0.056			
nal25ace10	330	1.20E-01 IV / 1	1.15E+02	2.03E+00	0.138	0.210	0.228	-0.072			
"	330	1.20E-01 IV / 1	1.12E+02	3.13E+00	0.088	0.210	0.228	-0.09754	5.92E+02	1.35E+02	-0.0245
nal25ace11	330	1.20E-01 IV / 2	1.12E+02	3.18E+00	0.098	0.151	0.173	-0.053			
				1.10E+02					5.30E+02		

o-NBAL in 17 mM acetate buffer				I=0.1	[Buffer]= 17 mM		o-nitrobenzyl alcohol				
nal17ace1	330	1.70E-01 I / 1	8.21E+01	1.52E+00	0.156	0.221	0.238	-0.06533			
"	330	1.70E-01 I / 1	7.97E+01	2.22E+00	0.075	0.221	0.238	-0.10475	3.62E+02	4.92E+01	-0.0413
nal17ace2	330	1.70E-01 I / 2	8.90E+01	2.12E+00	0.116	0.171	0.191	-0.055			
"	330	1.70E-01 I / 2	8.82E+01	2.47E+00	0.062	0.171	0.191	-0.08656	5.62E+02	1.37E+02	-0.0227
nal17ace3	330	1.70E-01 I / 3	9.53E+01	2.34E+00	0.061	0.125	0.145	-0.064			
"	330	1.70E-01 I / 3	9.06E+01	3.51E+00	0.048	0.125	0.145	-0.06604	3.69E+02	0	-0.0106
nal17ace4	320	1.70E-01 II / 1	8.73E+01	1.99E+00	0.155	0.222	0.241	-0.067			
"	320	1.70E-01 II / 1	8.66E+01	2.27E+00	0.081	0.222	0.241	-0.10853	5.57E+02	1.13E+02	-0.0320
nal17ace5	325	1.70E-01 II / 2	8.92E+01	3.64E+00	0.098	0.140	0.162	-0.042			
"	325	1.70E-01 II / 2	8.93E+01	4.48E+00	0.041	0.140	0.162	-0.06937	5.08E+02	1.29E+02	-0.0295

			8.69E+01						4.72E+02		
nal17ace6	410	1.50E-06 III / 1	1.01E+07	6.87E+04	0.095	0.006	0.113	0.088			
"	410	1.50E-06 III / 1	8.93E+06	1.62E+05	0.101	0.006	0.113	0.07546	3.93E+07	5.07E+06	0.0197
nal17ace7	430	1.50E-06 III / 3	9.13E+06	1.38E+05	0.038	0.003	0.075	0.035			
"	430	1.50E-06 III / 3	8.94E+06	2.46E+05	0.068	0.003	0.075	0.05328	3.73E+07	8.15E+06	0.0116
nal17ace8	430	1.50E-06 IV / 2	1.02E+07	7.39E+04	0.084	0.004	0.092	0.080			
"	430	1.50E-06 IV / 2	9.39E+06	1.59E+05	0.089	0.004	0.092	0.07344	3.90E+07	9.80E+06	0.0122
nal17ace9	420	1.50E-06 IV / 3	9.91E+06	7.61E+04	0.069	0.004	0.078	0.065			
"	420	1.50E-06 IV / 3	8.56E+06	2.38E+05	0.073	0.003	0.078	0.05432	3.04E+07	5.03E+06	0.0152
nal17ace10	420	1.50E-06 IV / 4	9.33E+06	2.57E+05	0.058	0.002	0.061	0.04481	4.33E+07	7.93E+06	0.0112
			9.03E+06						3.79E+07		

o-NBAL in 10 mM acetate buffer				I=0.1	[Buffer]=	10 mM			o-nitrobenzyl alcohol			
nal10ace1	470	2.00E-06 I / 1	1.01E+07	8.13E+04	0.082	0.004	0.097	0.079				
"	470	2.00E-06 I / 1	7.04E+06	1.69E+05	0.092	0.003	0.097	0.050	2.96E+07	1.69E+06	0.0390	
nal10ace2	430	2.00E-06 I / 2	6.78E+06	6.22E+04	0.049	0.005	0.118	0.045				
"	430	2.00E-06 I / 2	6.64E+06	8.26E+04	0.097	0.005	0.118	0.067	3.78E+07	2.63E+06	0.0252	
nal10ace3	410	2.00E-06 I / 3	6.48E+06	1.47E+05	0.075	0.004	0.083	0.048	2.67E+07	2.24E+06	0.0233	
nal10ace4	410	2.00E-06 II / 1	6.63E+06	8.42E+04	0.117	0.007	0.133	0.076	3.42E+07	1.94E+06	0.0340	
nal10ace5	490	2.00E-06 II / 2	9.83E+06	3.93E+05	0.015	0.002	0.043	0.013				
nal10ace6	400	2.00E-06 II / 3	6.72E+06	1.53E+05	0.022	0.004	0.063	0.018				
"	400	2.00E-06 II / 3	6.30E+06	1.60E+05	0.055	0.004	0.063	0.033	3.43E+07	3.41E+06	0.0175	
			6.62E+06						3.25E+07			
nal10ace7	320	2.10E-01 III / 1	6.59E+01	1.10E+00	0.152	0.243	0.262	-0.091				
"	320	2.10E-01 III / 1	6.32E+01	1.61E+00	0.074	0.243	0.262	-0.131	3.20E+02	5.60E+01	-0.0381	
nal10ace8	320	2.10E-01 III / 2	6.11E+01	1.91E+00	0.101	0.169	0.201	-0.068				
nal10ace9	330	2.10E-01 III / 3	6.56E+01	1.70E+00	0.065	0.118	0.133	-0.052				
nal10ace10	330	2.10E-01 IV / 1	6.46E+01	8.24E-01	0.117	0.190	0.201	-0.073				
"	330	2.10E-01 IV / 1	6.24E+01	1.23E+00	0.058	0.190	0.201	-0.104	3.13E+02	4.57E+01	-0.0277	
nal10ace11	330	2.10E-01 IV / 2	6.57E+01	1.03E+00	0.083	0.153	0.166	-0.071				
"	330	2.10E-01 IV / 2	6.33E+01	1.73E+00	0.043	0.154	0.166	-0.087	3.37E+02	6.80E+01	-0.0234	
			6.36E+01						3.23E+02			
			6.54E+01									

o-NBAL in 5 mM acetate buffer			I=0.1	[Buffer]= 5 mM					o-nitrobenzyl alcohol		
nal5ace1	410	2.70E-06 I / 3	4.56E+06	1.39E+05	0.027	0.004	0.079				

"	410	2.70E-06 I / 3	4.52E+06	1.69E+05	0.074	0.004	0.079	0.039373	2.54E+07	2.52E+06	0.0307
nal5ace2	430	2.20E-06 I / 5	4.56E+06	3.37E+05	0.055	0.002	0.060	0.030	1.75E+07	2.77E+06	0.0229
nal5ace3	320	2.70E-01 II / 1	4.35E+01	5.16E-01	0.157	0.225	0.237				
"	320	2.70E-01 II / 1	4.30E+01	7.52E-01	0.064	0.225	0.237	-0.125	1.78E+02	1.95E+01	-0.0355
nal5ace4	320	2.70E-01 II / 2	4.38E+01	7.91E-01	0.051	0.076	0.082				
"	320	2.70E-01 II / 2	3.85E+01	1.77E+00	0.021	0.076	0.082	-0.033	1.34E+02	1.38E+01	-0.0227
nal5ace5	330	2.70E-01 II / 3	4.33E+01	8.55E-01	0.074	0.118	0.133				
nal5ace6	330	2.70E-01 III / 1	4.60E+01	3.32E-01	0.127	0.207	0.217				
"	330	2.70E-01 III / 1	4.54E+01	4.83E-01	0.060	0.207	0.217	-0.128	2.17E+02	2.81E+01	-0.0200
nal5ace7	330	3.70E-01 III / 2	4.47E+01	1.11E+00	0.064	0.173	0.180	-0.092	1.53E+02	3.57E+01	-0.0166
nal5ace8	330	3.70E-01 III / 3	4.43E+01	8.29E-01	0.079	0.119	0.126				
			4.41E+01						1.83E+02		
nal5ace9	430	2.70E-06 IV / 1	4.74E+06	5.50E+04	0.134	0.005	0.134	0.074	2.66E+07	8.35E+05	0.0554
nal5ace10	410	2.00E-06 IV / 2	4.47E+06	8.00E+04	0.093	0.004	0.093	0.046	2.47E+07	8.93E+05	0.0430
nal5ace11	460	2.00E-06 IV / 3	4.65E+06	1.59E+05	0.060	0.002	0.061	0.027	2.29E+07	1.28E+06	0.0304
			4.59E+06						2.34E+07		

p[H⁺] = 4.56

[MeCOOH]/[NaOH] =

2.0

o-NBAL in 50 mM acetate buffer

l=0.1

[Buffer]= 50 mM

o-nitrobenzyl alcohol

File	λ /nm	Time range	Comments	$k(1)/s^{-1}$	error k(1)	A0	A_inf	A_max	A0-Ainf(1)	$k(2)/s^{-1}$	error k(2)	A0-Ainf(2)	A2/A1
nal50ac1	410	1.50E-06 I / 1		1.11E+07	6.27E+04	0.111	0.010	0.156	0.101				
nal50ac2	410	1.50E-06 I / 2		1.10E+07	1.01E+05	0.065	0.007	0.116	0.058				
nal50ac3	410	1.50E-06 I / 3		1.11E+07	8.37E+04	0.076	0.006	0.093	0.070				
"	410	1.50E-06 I / 3		1.06E+07	1.32E+05	0.047	0.006	0.093	0.041				
nal50ac4	450	1.50E-06 I / 4		1.13E+07	1.02E+05	0.064	0.003	0.084	0.061				
				1.11E+07									
nal50ac5	320	5.30E-06 II / 1		1.74E+07	3.55E+06	0.122	0.147	0.172	-0.024				
nal50ac6	320	1.70E-04 II / 1		1.64E+05	1.25E+04	0.148	0.135	0.155	0.013				
nal50ac7	320	3.50E-04 II / 2		1.61E+05	3.53E+04	0.091	0.083	0.116	0.008				
nal50ac8	330	5.30E-02 II / 4		3.39E+02	1.02E+01	0.063	0.090	0.098	-0.027				
nal50ac9	330	5.30E-02 II / 5		4.04E+02	1.88E+01	0.058	0.078	0.088	-0.020				
nal50ac10	320	7.40E-02 III / 1		3.40E+02	9.32E+00	0.161	0.218	0.234	-0.058				
nal50ac11	320	7.40E-02 III / 2		3.50E+02	1.72E+01	0.095	0.128	0.145	-0.032				
nal50ac12	320	7.40E-02 III / 3		4.11E+02	3.86E+01	0.066	0.088	0.106	-0.021				

nal50ac13	330	7.40E-02 III / 4	3.75E+02 3.43E+02	1.98E+01	0.069	0.092	0.103	-0.023
nal50ac14	450	8.30E-07 IV / 1	1.12E+07	4.55E+04	0.099	0.007	0.153	0.092
nal50ac15	450	1.00E-06 IV / 2	1.15E+07	5.87E+04	0.084	0.004	0.105	0.080
nal50ac16	410	1.00E-06 IV / 3	1.12E+07	6.24E+04	0.076	0.005	0.091	0.071

o-NBAL in 35 mM acet.buffer

I=0.1

35 mM

o-nitrobenzyl alcohol

nal35ac1	330	9.00E-02 0.5/5 180mJ I/	2.24E+02	3.35E+00	0.180	0.272	0.288	-0.092			
nal35ac2	330	7.50E-02 I / 2	2.26E+02	6.20E+00	0.086	0.181	0.193	-0.096			
"	330	7.50E-02 I / 2	2.26E+02	6.20E+00	0.086	0.181	0.193	-0.073135	1.46E+03	2.96E+02	-2.25E-02
nal35ac3	330	7.50E-02 I / 3	2.16E+02	7.71E+00	0.101	0.133	0.147	-0.033			
nal35ac4	320	8.10E-02 II / 1	2.37E+02	3.35E+00	0.197	0.299	0.313	-0.102			
nal35ac5	320	8.10E-02 II / 2	2.41E+02	7.32E+00	0.119	0.177	0.197	-0.058			
nal35ac6	330	8.10E-02 II / 3	2.50E+02 2.29E+02	1.06E+01	0.075	0.116	0.136	-0.041			
nal35ac7	320	1.10E-04 III / 1	6.12E+04	2.88E+03	0.129	0.114	0.142	0.015			
nal35ac8	410	2.00E-06 III / 2	8.56E+06	5.26E+04	0.083	0.007	0.105	0.076			
nal35ac9	410	2.00E-06 III / 3	8.31E+06	7.27E+04	0.056	0.006	0.078	0.050			
nal35ac10	470	2.00E-06 IV / 1	8.64E+06	1.00E+05	0.108	0.005	0.114	0.084509	4.25E+07	4.57E+06	1.87E-02
nal35ac11	410	2.00E-06 IV / 2	8.26E+06	5.55E+04	0.075	0.007	0.104	0.068			
nal35ac12	410	2.00E-06 IV / 3	8.67E+06 8.49E+06	6.37E+04	0.065	0.006	0.082	0.059			

o-NBAL in 25 mM acet.buffer

0.5/5 205mJ

I=0.1

25 mM

o-nitrobenzyl alcohol

nal25ac1	410	2.90E-06 I / 1	6.75E+06	6.31E+04	7.30E-02	1.04E-02	1.31E-01	0.063			
"	410	2.90E-06 I / 1	6.56E+06	0.00E+00	0.131	0.010	0.131	0.10227	3.47E+07	3.48E+06	1.80E-02
nal25ac2	410	2.10E-06 I / 2	6.68E+06	8.06E+04	8.76E-02	7.17E-03	9.27E-02	0.080	5.85E+07	1.11E+07	1.01E-02
"	410	2.10E-06 I / 2	6.72E+06	7.47E+04	5.32E-02	7.19E-03	9.27E-02	0.046			
nal25ac3	410	2.10E-06 I / 3	6.83E+06	6.60E+04	5.78E-02	6.38E-03	6.79E-02	0.051			
nal25ac4	450	2.10E-06 I / 4	6.98E+06 6.80E+06	9.72E+04	4.09E-02	3.44E-03	5.29E-02	0.037			
nal25ac5	320	3.50E-06 II / 1	1.57E+07	3.32E+06	1.20E-01	1.46E-01	1.70E-01	-0.026			
nal25ac6	320	1.20E-04 II / 1	4.74E+04	1.05E+03	1.40E-01	1.17E-01	1.49E-01	0.024			
nal25ac7	320	1.40E-04 II / 2	6.41E+04	3.21E+03	8.74E-02	7.19E-02	9.41E-02	0.015			
nal25ac8	320	6.40E-02 II / 3	1.99E+02	3.34E+00	8.06E-02	1.26E-01	1.37E-01	-0.045			

4.66E+07

nal25ac9	330	1.00E-01 II / 4	1.78E+02	5.46E+00	5.43E-02	8.86E-02	1.04E-01	-0.034
nal25ac10	320	1.00E-01 III / 1	1.87E+02	3.22E+00	1.38E-01	2.24E-01	2.45E-01	-0.086
"	320	1.00E-01 III / 1	1.79E+02	3.83E+00	1.56E-01	2.24E-01	2.45E-01	
nal25ac11	320	1.00E-01 III / 2	1.83E+02	6.24E+00	8.46E-02	1.28E-01	1.45E-01	
nal25ac12	330	1.00E-01 III / 3	1.86E+02	6.26E+00	6.32E-02	9.02E-02	9.99E-02	
nal25ac13	330	1.00E-01 III / 4	2.38E+02	1.61E+01	4.91E-02	6.65E-02	8.11E-02	
			1.86E+02					
nal25ac14	330	1.00E-01 IV / 1	1.88E+02	2.52E+00	1.21E-01	1.92E-01	2.02E-01	
nal25ac15	450	1.70E-06 IV / 2	6.91E+06	1.12E+05	0.038	0.004	0.063	
nal25ac16	450	1.70E-06 IV / 3	6.78E+06	1.06E+05	0.040	0.004	0.053	

o-NBAL in 17.5 mM acet.buffer

0.5/5 205mJ

I=0.1

17.5 mM

o-nitrobenzyl alcohol

nal17ac1	410	1.90E-06 I / 1	5.31E+06	5.81E+04	0.058	0.011	0.148				
"	410	1.90E-06 I / 1	5.39E+06	4.62E+04	0.137	0.011	0.148	0.102510	4.10E+07	3.66E+06	2.29E-02
nal17ac2	410	2.10E-06 I / 2	5.37E+06	5.56E+04	0.099	0.006	0.104	0.076792	4.41E+07	5.33E+06	1.56E-02
nal17ac3	410	2.10E-06 I / 3	5.45E+06	6.75E+04	0.069	0.005	0.070	0.055516	5.29E+07	1.16E+07	8.03E-03
nal17ac4	410	2.10E-06 I / 4	5.34E+06	6.37E+04	0.042	0.005	0.059				
			5.38E+06						4.16E+07		
nal17ac5	320	3.10E-06 II / 1	1.21E+07	5.80E+06	0.125	0.142	0.167				
nal17ac6	320	1.70E-04 II / 1	3.51E+04	9.53E+02	0.134	0.110	0.146				
nal17ac7	330	1.70E-04 II / 2	4.91E+04	2.09E+03	0.067	0.054	0.073				
nal17ac8	330	2.60E-01 II / 3	1.48E+02	4.22E+00	0.079	0.120	0.129				
nal17ac9	330	2.60E-01 II / 4	1.04E+02	5.75E+00	0.068	0.087	0.973				
nal17ac10	320	2.60E-01 III / 1	1.49E+02	2.56E+00	0.146	0.221	0.231				
nal17ac11	320	1.80E-01 III / 2	1.51E+02	4.56E+00	0.096	0.143	0.156				
nal17ac12	330	1.80E-01 III / 3	1.43E+02	4.33E+00	0.072	0.103	0.112				
nal17ac13	330	1.80E-01 III / 4	1.59E+02	7.31E+00	0.056	0.080	0.091				
			1.48E+02								
nal17ac14	410	3.40E-06 IV / 1	5.37E+06	4.81E+04	0.130	0.010	0.140	0.099920	4.50E+07	5.30E+06	2.00E-02
nal17ac15	410	2.60E-06 IV / 2	5.40E+06	7.07E+04	0.089	0.007	0.098	0.069279	3.62E+07	5.97E+06	0.013
nal17ac16	410	2.60E-06 IV / 3	5.34E+06	8.00E+04	0.066	0.005	0.068	0.051482	5.43E+07	1.06E+07	9.48E-03

o-NBAL in 10 mM acet.buffer

205mJ

I=0.1

10 mM

o-nitrobenzyl alcohol

nal10ac1	410	2.70E-06 I / 1	3.83E+06	2.34E+04	0.076	0.005	0.076	0.051	3.22E+07	1.22E+06	2.01E-02
----------	-----	----------------	----------	----------	-------	-------	-------	-------	----------	----------	----------

nal10ac2	410	2.70E-06 I / 2	3.76E+06	3.32E+04	0.106	0.007	0.112	0.069	3.08E+07	1.55E+06	2.92E-02
nal10ac3	410	2.70E-06 I / 3	3.74E+06	4.36E+04	0.084	0.006	0.085	0.054	3.74E+07	4.36E+04	2.41E-02
nal10ac4	450	2.70E-06 I / 4	3.81E+06	5.71E+04	0.064	0.003	0.066	0.040	3.24E+07	2.32E+06	2.06E-02
			3.82E+06						3.17E+07		
nal10ac5	320	3.40E-04 II / 1	2.83E+04	6.44E+02	0.135	0.109	0.140				
nal10ac6	320	5.40E-06 II / 1	2.23E+07	1.05E+07	0.120	0.136	0.160				
nal10ac7	320	8.00E-04 II / 2	8.20E+04	2.24E+04	0.086	0.079	0.098				
nal10ac8	320	2.10E-01 II / 3	1.03E+02	2.18E+00	0.067	0.106	0.114				
nal10ac9	330	2.10E-01 II / 4	9.60E+01	1.54E+00	0.067	0.101	0.107				
nal10ac10	330	2.40E-01 III / 2	9.62E+01	3.51E+00	0.058	0.091	0.104				
nal10ac11	330	2.40E-01 III / 3	9.62E+01	1.86E+00	0.059	0.094	0.101				
nal10ac12	330	2.40E-01 III / 4	1.08E+02	3.29E+00	0.046	0.074	0.082				
			1.00E+02								
nal10ac13	450	2.30E-06 IV / 1	3.90E+06	2.54E+04	0.151	0.005	0.152	0.092	3.07E+07	7.96E+05	5.35E-02
nal10ac14	450	2.30E-06 IV / 2	3.89E+06	3.35E+04	0.113	0.004	0.111	0.069	3.04E+07	1.02E+06	4.06E-02
nal10ac15	410	2.30E-06 IV / 3	3.80E+06	3.91E+04	0.087	0.005	0.094	0.059	2.84E+07	1.69E+06	2.31E-02

o-NBAL in 5 mM acet.buffer

o-NBAL in 5 mM acet.buffer			I=0.1		5 mM		H2O		o-nitrobenzyl alcohol		
nal5ac1	410	5.20E-06 I / 1	2.41E+06	2.10E+04	0.050	0.009	0.152	0.041084			
"	410	5.20E-06 I / 1	2.45E+06	1.84E+04	0.141	0.009	0.152	0.073336	2.35E+07	5.91E+05	5.90E-02
nal5ac2	410	5.20E-06 I / 2	2.42E+06	2.40E+04	0.091	0.006	0.104	0.049928	2.84E+07	1.18E+06	3.51E-02
nal5ac3	410	6.00E-07 I / 2	2.46E+06	0.00E+00	0.094	0.006	0.105	0.052471	3.16E+07	1.11E+06	3.55E-02
nal5ac4	430	6.00E-07 I / 3	2.44E+06	0.00E+00	0.079	0.003	0.086	0.046387	2.69E+07	1.14E+06	2.99E-02
nal5ac5	430	3.50E-06 I / 3	2.59E+06	3.05E+04	0.077	0.004	0.085	0.045013	2.70E+07	1.35E+06	2.79E-02
			2.47E+06						2.61E+07		
nal5ac6	320	3.30E-04 II / 1	1.58E+04	1.87E+02	0.125	0.094	0.135				
nal5ac7	390	4.20E-06 II / 2	2.42E+06	4.46E+04	0.077	0.007	0.078	0.033931	2.40E+07	9.77E+05	3.50E-02
nal5ac8	410	4.20E-06 II / 3	2.47E+06	3.33E+04	0.070	0.005	0.074	0.038263	2.76E+07	1.34E+06	2.74E-02
			5.67E+01	6.79E+00							
nal5ac9	320	3.00E-01 III / 1	4.93E+01	7.08E-01	0.149	0.352	0.358	-0.137190	1.67E+02	7.765	-6.58E-02
nal5ac10	320	1.00E+00 III / 2	6.46E+01	8.88E-01	0.145	0.235	0.242				
nal5ac11	330	1.00E+00 III / 3	6.73E+01	3.15E+00	0.110	0.129	0.134				
"	330	1.00E+00 III / 3	6.43E+01	1.26E+00	0.089	0.129	0.134				
nal5ac12	330	3.00E-01 IV / 1	5.73E+01	6.63E-01	0.193	0.265	0.272				
"	330	1.00E+00 IV / 1	5.37E+01	6.47E-01	0.195	0.266	0.272				
nal5ac13	330	4.00E-01 IV / 2	5.70E+01	8.99E-01	0.122	0.166	0.173				

nal5ac14	330	4.00E-01 IV / 3	4.78E+01	1.74E+00	0.104	0.127	0.137
"	330	1.80E-01 IV / 3	6.02E+01	1.24E+00	0.081	0.126	0.137

p[H⁺] = 5.07

[MeCOOH]/[NaOH] = 1.32

o-NBAL in 50 mM acet.buffer

I=0.1 [Buffer]= 50 mM

o-nitrobenzyl alcohol

File	λ /nm	Time range	Comments	$k(1)/s^{-1}$	error k(1)	A0	A_inf	A_max	A0-Ainf(1)	$k(2)/s^{-1}$	error k(2)	A0-Ainf(2)	A2/A1
nal5ac1	410	3.60E-06 I / 1		5.14E+06	2.35E+04	0.131	0.011	0.147	0.120				
"	410	3.60E-06 I / 1		5.01E+06	6.46E+04	0.053	0.011	0.147	0.042				
nal5ac2	410	2.10E-06 I / 2		5.10E+06	1.00E+05	0.030	0.009	0.111	0.021				
nal5ac3	410	2.10E-06 I / 3		5.17E+06	3.43E+04	0.066	0.006	0.076	0.060				
nal5ac4	450	2.10E-06 I / 4		5.10E+06	4.71E+04	0.047	0.004	0.055	0.043				
nal5ac5	450	2.10E-06 I / 5		5.08E+06	5.81E+04	0.038	0.004	0.044	0.034				
				5.10E+06									
nal5ac6	320	3.70E-06 II / 1		1.09E+07	1.66E+06	0.133	0.162	0.184	-0.028				
nal5ac7	320	1.80E-04 II / 1		8.66E+04	6.21E+03	0.160	0.149	0.167	0.011				
nal5ac8	310	1.00E-04 II / 2		7.95E+04	7.44E+03	0.092	0.077	0.107	0.015				
nal5ac9	310	7.10E-06 II / 3		4.78E+07	1.06E+08	0.092	0.091	0.133	0.001				
nal5ac10	330	7.10E-06 II / 4		3.73E+07	1.92E+07	0.054	0.066	0.086	-0.013				
nal5ac11	330	5.20E-05 II / 4		1.41E+05	1.84E+04	0.066	0.058	0.077	0.007				
nal5ac12	330	9.00E-03 II / 5		4.44E+02	3.06E+01	0.051	0.097	0.104	-2.40E-02	2.34E+03	2.03E+02	-2.23E-02	0.9303
nal5ac13	330	3.00E-02 II / 5		7.30E+02	5.23E+01	0.043	0.058	0.069	-0.014				
				8.31E+04									
nal5ac14	320	2.80E-02 III / 1		4.37E+02	1.04E+01	0.205	0.236	0.247	-0.032				
"	320	2.80E-02 III / 1		4.46E+02	9.17E+00	0.109	0.236	0.247	-7.34E-02	2.58E+03	1.53E+02	-5.42E-02	0.7387
nal5ac15	320	2.80E-02 III / 2		4.60E+02	2.38E+01	0.075	0.142	0.155	-3.87E-02	2.74E+03	4.04E+02	-2.86E-02	0.7392
nal5ac16	330	2.80E-02 III / 3		4.79E+02	1.77E+01	0.076	0.094	0.102	-0.018				
nal5ac17	330	2.80E-02 III / 4		4.60E+02	0E+00	0.048	0.075	0.078	-8.87E-03	1.17E+03	9.17E+01	-1.84E-02	2.0797
				4.53E+02						2.55E+03			
nal5ac18	330	2.80E-02 IV / 1		4.96E+02	1.19E+01	0.181	0.206	0.213	-0.025				
nal5ac19	410	3.60E-06 IV / 2		5.08E+06	3.74E+04	0.072	0.006	0.084	0.066				
nal5ac20	410	3.60E-06 IV / 3		4.95E+06	4.46E+04	0.062	0.006	0.068	0.056				

o-NBAL in 35 mM acet.buffer

			I=0.1	35 mM				o-nitrobenzyl alcohol			
nal35ac1	410	6.00E-06 I / 1	3.99E+06	1.33E+04	0.142	0.011	0.164	0.131			
"	410	6.00E-06 I / 1	3.90E+06	5.22E+04	0.047	0.011	0.164	0.035			
nal35ac2	390	6.00E-06 I / 2	3.65E+06	2.47E+04	0.072	0.006	0.084	0.066			
"	390	6.00E-06 I / 2	3.87E+06	4.83E+04	0.058	0.007	0.084	0.050			
nal35ac3	450	3.40E-06 I / 3	3.89E+06	2.37E+04	0.068	0.004	0.088	0.064			
			3.89E+06								
nal35ac4	320	8.30E-05 II / 1	4.81E+04	3.62E+03	0.147	0.136	0.162	0.011			
nal35ac5	410	2.60E-06 II / 2	3.91E+06	1.93E+04	0.084	0.006	0.114	0.077			
nal35ac6	320	9.30E-02 III / 1	3.22E+02	7.59E+00	0.208	0.333	0.342	-0.096793	1.77E+03	3.03E+02	-2.88E-02
nal35ac7	320	9.30E-02 III / 2	3.02E+02	1.28E+01	0.173	0.201	0.214	-0.028			
"	320	9.30E-02 III / 2	2.78E+02	2.42E+01	0.125	0.201	0.214	-0.045392	9.16E+02	2.11E+02	-2.98E-02
nal35ac8	330	9.30E-02 IV / 1	3.16E+02	5.51E+00	0.140	0.255	0.262	-0.082911	2.05E+03	2.14E+02	-3.29E-02
nal35ac9	330	9.30E-02 IV / 2	3.37E+02	6.58E+00	0.108	0.183	0.190	-0.061111	2.75E+03	6.11E+02	-1.40E-02
nal35ac10	330	9.30E-02 IV / 3	3.11E+02	1.45E+01	0.121	0.137	0.143	-0.016			
			3.22E+02						1.91E+03		

o-NBAL in 25 mM acet.buffer

			I=0.1	25 mM				o-nitrobenzyl alcohol			
nal25ac1	410	1.30E-06 I / 1	3.08E+06	2.30E+04	0.131	0.012	0.136	1.08E-01	5.18E+07	7.43E+06	1.01E-02 0.0937
nal25ac2	410	3.40E-06 I / 1	3.07E+06	1.37E+04	0.130	0.013	0.136	1.08E-01	5.29E+07	8.66E+06	9.91E-03 0.0917
nal25ac3	410	3.40E-06 I / 2	3.08E+06	2.12E+04	0.089	0.009	0.091	7.38E-02	4.37E+07	1.27E+07	6.65E-03 0.0902
nal25ac5	410	1.00E-06 I / 2	3.03E+06	4.91E+04	0.089	0.009	0.092	7.33E-02	4.20E+07	1.31E+07	6.90E-03 0.0942
nal25ac4	410	2.90E-06 I / 3	3.07E+06	2.31E+04	0.056	0.007	0.061	0.049			
nal25ac6	450	2.90E-06 I / 4	3.03E+06	4.82E+04	0.026	0.004	0.043	0.022			
"	450	2.90E-06 I / 4	3.04E+06	3.53E+04	0.041	0.004	0.043	3.30E-02	1.21E+08	6.01E+07	3.72E-03 0.1127
nal25ac7	450	1.20E-06 I / 4	3.07E+06	6.81E+04	0.041	0.004	0.043	3.32E-02	8.08E+07	4.08E+07	3.22E-03 0.0970
			3.08E+06	5.84E+04					4.77E+07		
nal25ac8	320	2.60E-06 II / 1	1.37E+07	2.19E+06	0.131	0.152	0.166	-0.021			
nal25ac9	320	1.50E-04 II / 1	2.83E+04	3.20E+02	0.149	0.120	0.154	0.029			
nal25ac10	320	1.50E-04 II / 2	4.06E+04	7.52E+02	0.109	0.086	0.114	0.022			
nal25ac11	320	1.50E-04 II / 3	4.14E+04	1.60E+03	0.078	0.065	0.085	0.013			
nal25ac12	320	5.00E-02 II / 4	3.01E+02	6.14E+00	0.063	0.093	0.102	-0.031			
nal25ac13	320	1.30E-01 III / 1	2.43E+02	4.92E+00	0.147	0.210	0.221	-0.063			
nal25ac14	320	1.00E-01 III / 2	2.31E+02	6.67E+00	0.095	0.133	0.143	-0.037			

nal25ac15	320	1.00E-01 III / 3	2.74E+02	1.11E+01	0.064	0.092	0.104	-0.027				
nal25ac16	330	1.00E-01 III / 4	3.10E+02	1.71E+01	0.049	0.062	0.069	-0.013				
nal25ac17	330	1.00E-01 III / 5	3.21E+02	2.58E+01	0.042	0.051	0.058	-0.010				
			2.50E+02									
nal25ac18	330	1.00E-01 IV / 1	2.57E+02	6.41E+00	0.150	0.183	0.190	-0.032				
"	330	1.00E-01 IV / 1	2.71E+02	3.58E+00	0.120	0.183	0.190	-0.062				
nal25ac19	450	3.50E-06 IV / 2	3.24E+06	2.77E+04	0.053	0.005	0.073	0.048				
"	450	3.50E-06 IV / 2	3.24E+06	3.29E+04	0.067	0.005	0.073	5.6094E-02	4.23E+07	1.18E+07	5.56E-03	
nal25ac20	450	3.50E-06 IV / 3	3.20E+06	3.42E+04	0.041	0.004	0.048					
nal25ac21	410	3.50E-06 IV / 4	3.01E+06	7.62E+04	0.021	0.006	0.038					
o-NBAL in 17.5 mM acet.buffer			I=0.1		17.5 mM			o-nitrobenzyl alcohol				
nal175ac1	410	1.30E-06 I / 1	2.34E+06	2.29E+04	0.154	0.010	0.160	1.21E-01	4.61E+07	3.15E+06	2.33E-02	0.1928
nal175ac2	410	4.40E-06 I / 1	2.34E+06	9.36E+03	0.155	0.010	0.160	1.21E-01	4.31E+07	3.05E+06	2.41E-02	0.1991
nal175ac3	410	4.40E-06 I / 2	2.37E+06	1.30E+04	0.105	0.006	0.107	8.54E-02	4.71E+07	5.90E+06	1.35E-02	0.1579
nal175ac4	410	1.10E-06 I / 2	2.37E+06	3.91E+04	0.104	0.007	0.108	8.45E-02	5.07E+07	6.91E+06	1.21E-02	0.1428
nal175ac5	410	1.10E-06 I / 3	2.27E+06	5.46E+04	0.079	0.004	0.081	6.52E-02	3.91E+07	6.63E+06	9.23E-03	0.1416
nal175ac6	410	3.40E-06 I / 3	2.36E+06	1.75E+04	0.078	0.005	0.081	6.48E-02	4.40E+07	8.20E+06	8.59E-03	0.1325
nal175ac7	450	3.40E-06 I / 4	2.42E+06	2.41E+04	0.059	0.004	0.064	4.82E-02	3.22E+07	6.77E+06	6.76E-03	0.1401
			2.45E+06						4.50E+07			
nal175ac8	320	1.50E-04 II / 1	2.47E+04	4.14E+02	0.157	0.130	0.162	0.027				
nal175ac9	320	6.40E-06 II / 1	1.06E+07	2.15E+06	0.137	0.157	0.178	-0.020				
nal175ac10	320	6.40E-06 II / 2	2.25E+07	1.32E+07	0.091	0.104	0.143	-0.014				
nal175ac11	320	1.20E-04 II / 2	4.30E+04	1.79E+03	0.102	0.084	0.111	0.018				
nal175ac12	320	1.20E-01 II / 3	2.33E+02	2.49E+01	0.089	0.099	0.109	-0.010				
"	320	1.20E-01 II / 3	2.27E+02	7.33E+00	0.065	0.099	0.109	-0.034				
nal175ac13	320	1.20E-01 II / 4	2.30E+02	7.37E+00	0.066	0.086	0.091	-0.020				
			2.04E+02									
nal175ac14	320	1.90E-01 III / 1	1.99E+02	5.29E+00	0.138	0.195	0.209	-0.056				
nal175ac15	320	1.10E-01 III / 1	2.12E+02	4.90E+00	0.125	0.194	0.211	-0.070				
nal175ac16	320	1.10E-01 III / 2	2.01E+02	1.10E+01	0.071	0.109	0.131	-0.038				
nal175ac17	330	1.10E-01 III / 3	2.25E+02	8.70E+00	0.058	0.092	0.105	-0.034				
nal175ac18	330	1.10E-01 III / 4	2.27E+02	1.07E+01	0.052	0.076	0.086	-0.024				
nal175ac19	450	4.30E-06 IV / 1	2.48E+06	9.77E+03	0.157	0.006	0.161	0.118580	3.83E+07	1.84E+06	3.20E-02	0.2695
nal175ac20	450	1.00E-06 IV / 1	2.64E+06	3.31E+04	0.158	0.009	0.162	0.118180	4.56E+07	2.31E+06	3.06E-02	0.2587

nal175ac21	450	1.00E-06 IV / 2	2.62E+06	4.90E+04	0.109	0.007	0.111	0.083639	4.36E+07	3.92E+06	1.81E-02	0.2169
nal175ac22	450	3.20E-06 IV / 2	2.51E+06	1.34E+04	0.108	0.005	0.110	0.083398	4.67E+07	3.58E+06	1.93E-02	0.2319
nal175ac23	410	3.20E-06 IV / 3	2.40E+06	1.62E+04	0.078	0.006	0.080	0.064983	4.25E+07	9.67E+06	6.53E-03	0.1005
nal175ac24	410	3.20E-06 IV / 3	2.39E+06	4.35E+04	0.078	0.006	0.083	0.064851	4.71E+07	1.12E+07	6.40E-03	0.0987

o-NBAL in 12.5 mM acet.buffer

I=0.1

12.5 mM

o-nitrobenzyl alcohol

nal12ac1	410	5.00E-06 I / 1	1.88E+06	1.54E+04	0.085	0.011	0.167					
"	410	5.00E-06 I / 1	1.82E+06	7.18E+03	0.165	0.010	0.167	1.14E-01	3.22E+07	1.17E+06	4.12E-02	
nal12ac2	410	4.30E-06 I / 2	1.83E+06	2.05E+04	0.062	0.006	0.118					
"	410	4.30E-06 I / 2	1.81E+06	8.85E+03	0.112	0.006	0.118	7.98E-02	3.81E+07	2.00E+06	2.59E-02	
nal12ac3	410	4.30E-06 I / 3	1.81E+06	2.51E+04	0.054	0.005	0.091					
"	410	4.30E-06 I / 3	1.79E+06	1.06E+04	0.090	0.005	0.091	6.55E-02	3.47E+07	2.31E+06	1.95E-02	
			1.82E+06						3.37E+07			
nal12ac4	390	4.30E-06 II / 1	1.82E+06	1.09E+04	0.113	0.008	0.115					
nal12ac5	390	7.00E-07 II / 1	1.88E+06	0.00E+00	0.114	0.010	0.117	7.14E-02	3.58E+07	9.20E+05	3.31E-02	
nal12ac6	470	7.00E-07 II / 2	1.77E+06	0.00E+00	0.075	0.001	0.081	4.41E-02	2.78E+07	6.25E+05	3.03E-02	
nal12ac7	470	4.40E-06 II / 2	1.83E+06	2.80E+04	0.031	0.003	0.082					
nal12ac8	330	1.80E-04 III / 1	2.14E+04	4.60E+02	0.147	0.118	0.151					
nal12ac9	320	6.30E-02 III / 3	1.41E+02	2.56E+00	0.062	0.142	0.148	-5.71E-02	7.76E+02	7.01E+01	-2.26E-02	
nal12ac10	330	1.80E-01 III / 4	1.38E+02	3.03E+00	0.093	0.118	0.124					
"	330	1.80E-01 III / 4	1.37E+02	2.80E+00	0.066	0.118	0.124	-4.34E-02	1.16E+03	3.13E+02	-8.85E-03	
			1.39E+02						8.39E+02			
nal12ac11	330	1.80E-01 IV / 1	1.45E+02	1.95E+00	0.207	0.273	0.284					
"	330	1.80E-01 IV / 1	1.44E+02	2.33E+00	0.109	0.273	0.284	-1.22E-01	7.22E+02	6.99E+01	-4.24E-02	
nal12ac12	330	1.80E-01 IV / 2	1.36E+02	3.11E+00	0.151	0.192	0.201					
"	330	1.80E-01 IV / 2	1.34E+02	3.31E+00	0.090	0.192	0.201	-8.01E-02	7.02E+02	1.32E+02	-2.25E-02	
nal12ac13	330	1.80E-01 IV / 3	1.40E+02	2.24E+00	0.090	0.141	0.149					

o-NBAL in 10 mM acet.buffer

I=0.1

10 mM

o-nitrobenzyl alcohol

nal1ac1	410	1.50E-05 I / 1	1.47E+06	9.90E+03	0.064	0.010	0.162	0.053				
"	410	1.50E-05 I / 1	1.52E+06	6.94E+03	0.130	0.010	0.162	0.099	2.82E+07	2.20E+06	2.10E-02	0.2134
nal1ac2	410	7.10E-06 I / 1										
nal1ac3	410	1.60E-06 I / 1	1.53E+06	0.00E+00	0.147	0.010	0.152	0.097	2.97E+07	1.07E+06	4.06E-02	0.4186
nal1ac4	410	1.60E-06 I / 2	1.57E+06	0.00E+00	0.097	0.007	0.105	0.068	3.59E+07	2.57E+06	2.18E-02	0.3191
nal1ac5	410	6.40E-06 I / 2	1.54E+06	9.51E+03	0.101	0.006	0.104	0.069	3.23E+07	1.98E+06	2.61E-02	0.3777

nal1ac6	410	6.40E-06 I / 3	1.54E+06	1.20E+04	0.071	0.005	0.076	0.053	3.94E+07	5.06E+06	1.32E-02	0.2496
-	410	1.10E-06 I / 3	1.53E+06	8.10E+04	0.076	0.005	0.077	5.39E-02	4.17E+07	4.63E+06	1.73E-02	0.3205
nal1ac7	410	1.10E-06 I / 4	1.50E+06	0.00E+00	0.060	0.002	0.064	4.25E-02	3.09E+07	3.03E+06	1.52E-02	0.3565
nal1ac8	450	4.40E-06 I / 4	1.57E+06	1.52E+04	0.059	0.003	0.062	4.11E-02	3.01E+07	2.68E+06	1.43E-02	0.3476
nal1ac9	450	4.40E-06 I / 5	1.57E+06	1.90E+04	4.62E-02	3.05E-03	5.00E-02	3.35E-02	2.94E+07	3.90E+06	9.68E-03	0.2887
nal1ac10	450	1.20E-06 I / 5	1.56E+06	1.14E+05	4.81E-02	2.59E-03	5.10E-02	3.48E-02	3.03E+07	5.07E+06	1.07E-02	
			1.53E+06						3.09E+07			
nal1ac11	320	2.00E-06 II / 1	6.95E+06	9.96E+05	1.31E-01	1.50E-01	1.71E-01	-0.019				
nal1ac12	320	9.10E-05 II / 1	2.08E+04	4.42E+02	1.49E-01	1.13E-01	1.54E-01	0.035				
nal1ac13	320	1.70E-04 II / 2	3.27E+04	1.09E+03	1.02E-01	7.80E-02	1.10E-01	0.024				
nal1ac14	320	6.30E-06 II / 2	1.37E+07	5.60E+06	7.82E-02	1.03E-01	1.39E-01	-0.024				
nal1ac15	330	1.90E-04 II / 3	4.05E+04	1.56E+03	6.30E-02	4.85E-02	6.97E-02	0.014				
nal1ac16	330	1.90E-04 II / 4	3.34E+04	2.45E+03	5.27E-02	4.42E-02	5.85E-02	0.009				
nal1ac17	320	9.40E-02 III / 1	1.32E+02	2.10E+00	9.41E-02	2.21E-01	2.29E-01	-9.03E-02	5.99E+02	4.54E+01	-3.63E-02	
nal1ac18	320	2.10E-01 III / 2	1.39E+02	4.24E+00	8.51E-02	1.21E-01	1.31E-01					
nal1ac19	330	2.10E-01 III / 3	1.43E+02	5.60E+00	7.83E-02	9.65E-02	1.03E-01					
nal1ac20	330	2.80E-01 III / 4	1.41E+02	8.93E+00	5.91E-02	7.59E-02	8.57E-02					
			1.36E+02									
nal1ac21	450	6.00E-06 IV / 1	1.61E+06	8.62E+03	1.30E-01	5.59E-03	1.40E-01	8.45E-02	2.72E+07	1.03E+06	3.96E-02	0.4690
nal1ac22	450	1.00E-06 IV / 1	1.53E+06	0.00E+00	1.37E-01	2.99E-03	1.42E-01	8.76E-02	2.69E+07	9.66E+05	4.62E-02	0.5269
nal1ac23	450	1.00E-06 IV / 2	1.74E+06	1.03E+05	8.97E-02	6.24E-03	9.22E-02	5.71E-02	3.14E+07	2.34E+06	2.64E-02	0.4618
nal1ac24	450	4.00E-06 IV / 2	1.59E+06	1.12E+04	9.29E-02	4.15E-03	9.23E-02	5.88E-02	2.82E+07	1.17E+06	2.99E-02	0.5076
nal1ac25	450	4.00E-06 IV / 3	1.60E+06	1.46E+04	6.14E-02	3.48E-03	6.83E-02	4.41E-02	3.13E+07	2.81E+06	1.38E-02	0.3135
nal1ac26	410	4.00E-06 IV / 4	1.52E+06	1.50E+04	4.84E-02	4.56E-03	5.19E-02	3.77E-02	5.14E+07	1.21E+07	6.11E-03	0.1620
nal1ac27	410	1.30E-06 IV / 4	1.41E+06	8.40E+04	5.18E-02	3.14E-03	5.27E-02	3.98E-02	4.59E+07	9.70E+06	8.93E-03	0.2244
o-NBAL in 7.5 mM acet.buffer				I=0.1	7.5 mM			o-nitrobenzyl alcohol				
nal7ac1	330	1.30E-01 I / 1	1.01E+02	9.62E-01	0.115	0.295	0.304	-0.136	5.60E+02	3.46E+01	-4.43E-02	0.3262
nal7ac2	330	1.70E-01 I / 2	9.96E+01	1.69E+00	0.085	0.192	0.198	-0.083	4.15E+02	4.53E+01	-2.42E-02	0.2931
nal7ac3	320	1.70E-01 II / 1	1.04E+02	1.27E+00	1.42E-01	3.46E-01	3.56E-01	-1.44E-01	5.03E+02	3.01E+01	-5.97E-02	0.4140
nal7ac4	320	4.00E-03 II / 1	1.01E+02	0.00E+00	1.33E-01	4.99E-01	2.29E-01	-3.87E-01	3.46E+04	1.37E+04	2.15E-02	-0.0556
nal7ac5	320	2.70E-01 II / 2	8.48E+01	2.14E+00	1.82E-01	2.13E-01	2.21E-01					
"	320	2.70E-01 II / 2	1.04E+02	2.28E+00	1.08E-01	2.12E-01	2.21E-01	-8.33E-02	5.84E+02	1.04E+02	-2.05E-02	0.2458
			1.02E+02						5.16E+02			