Electronic Supplementary Information (ESI)

1. Job's plots

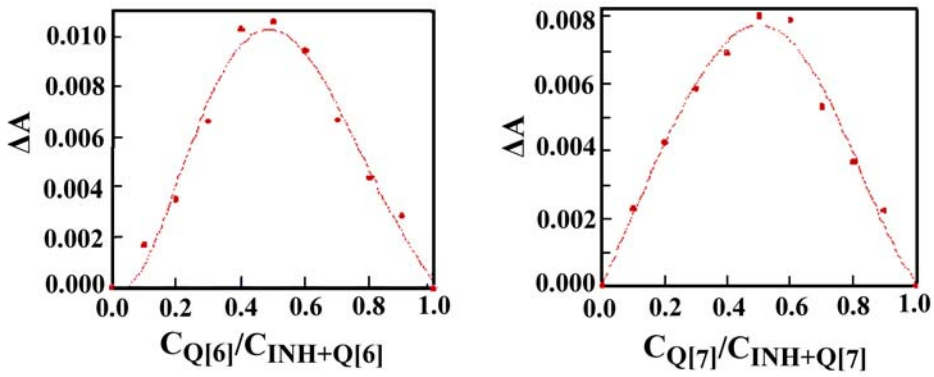


Fig. S1 Job's plots of the interaction between **INH** and cucurbiturils

2. ^{1}H NMR titrations

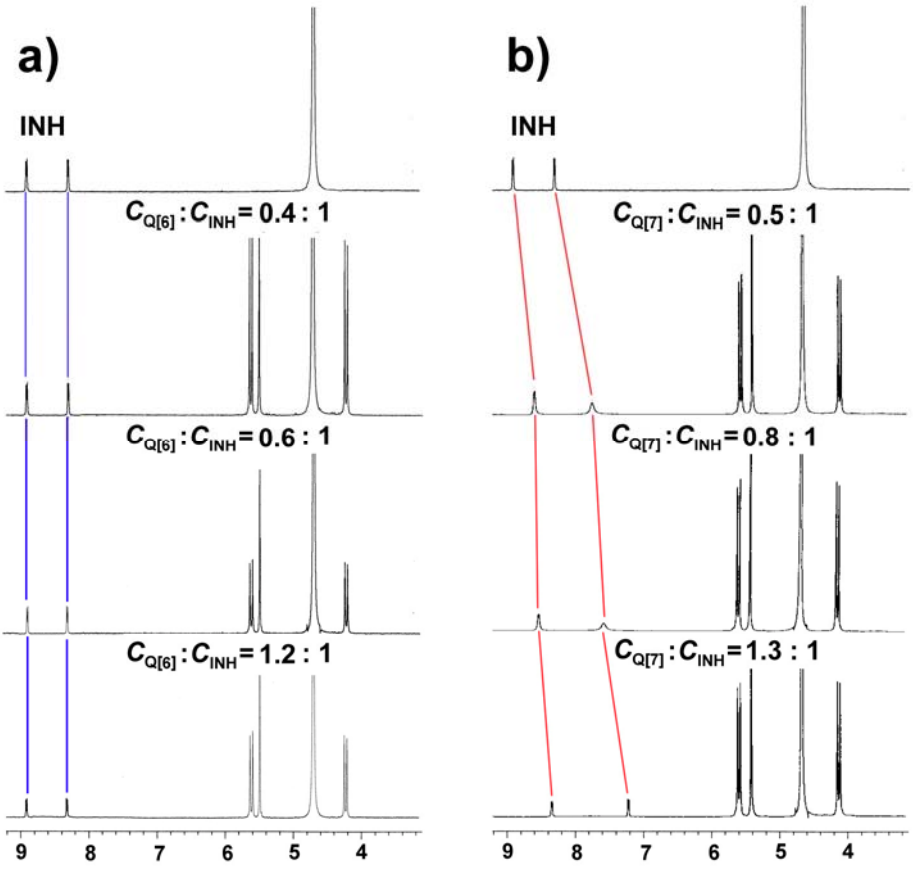
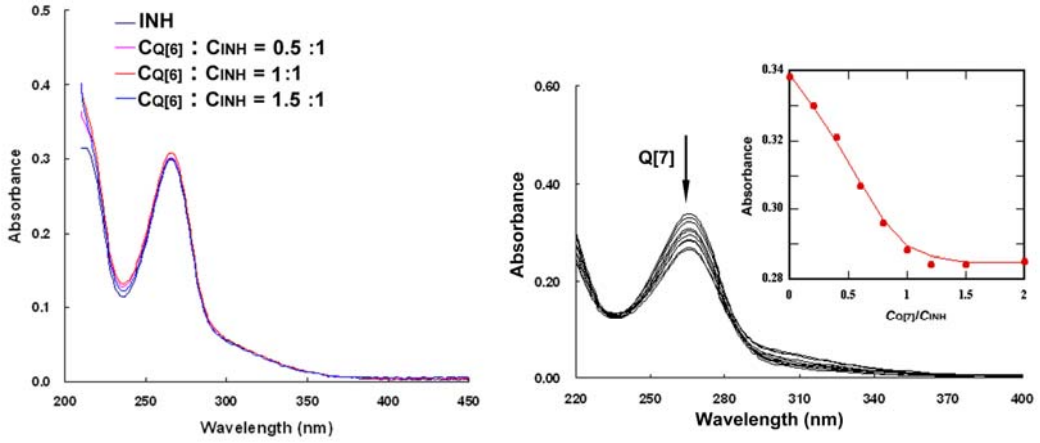


Fig. S2 ^{1}H NMR titrations of interactions between **INH** and Qs at pD ≈ 2

3. UV-vis titrations

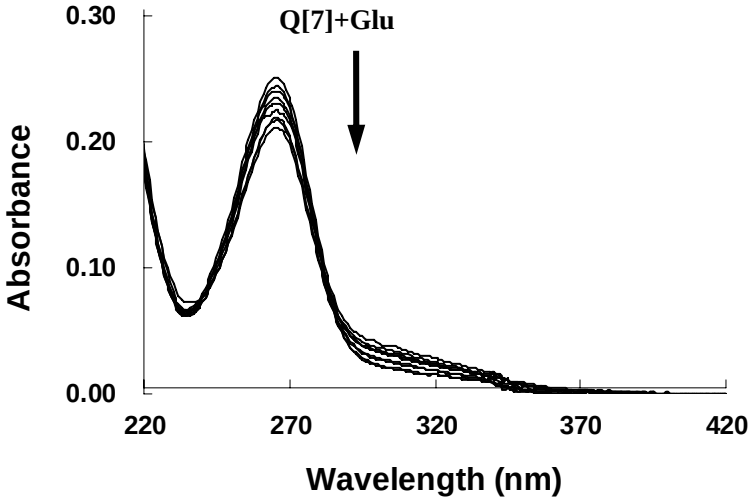


A **B**

Fig. S3 Electronic absorption spectra of **INH** in the presence of increasing concentrations of **A**) Q[6] and **B**) Q[7] at pH = 2, and corresponding absorbance vs NQ[6]/N**INH** curve (inset) at λ_{max} = 264 nm.

Competition titration experimentation

Q[7] and the glutamic acid (Glu) was dissolved in water with a 1:1 host:guest ratio, and adjusted to pH=2 by the addition of HCl to give solution A. **INH** solutions were prepared with a fixed concentration of 5.0 $\times 10^{-5}$ mol·L^{-1}, and the samples of these solutions with the solution A to give solutions with a solution A:**INH** ratio of 0, 0.25, 0.5, 0.8, 1.0 and so on. The competition titration has been recorded at λ_{max} = 264 nm.



C

Fig. S4 Electronic absorption spectra of **INH** in the presence of increasing concentrations of the solution **A** at pH = 2

4. Potential energy curves

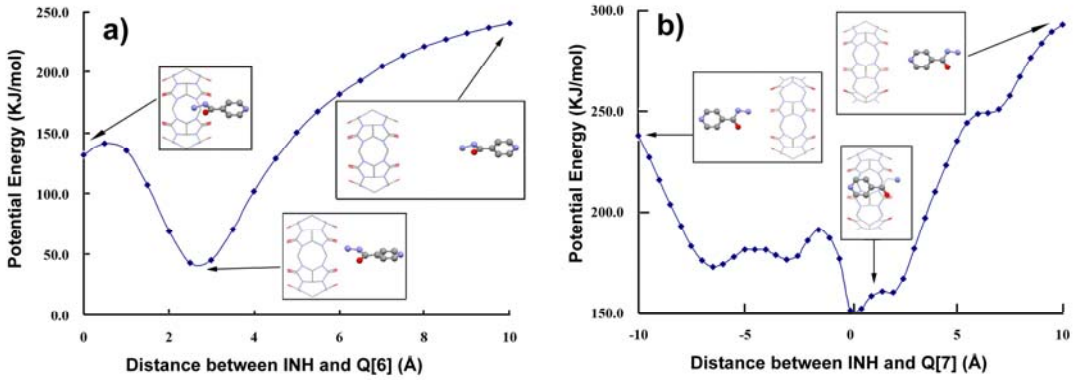
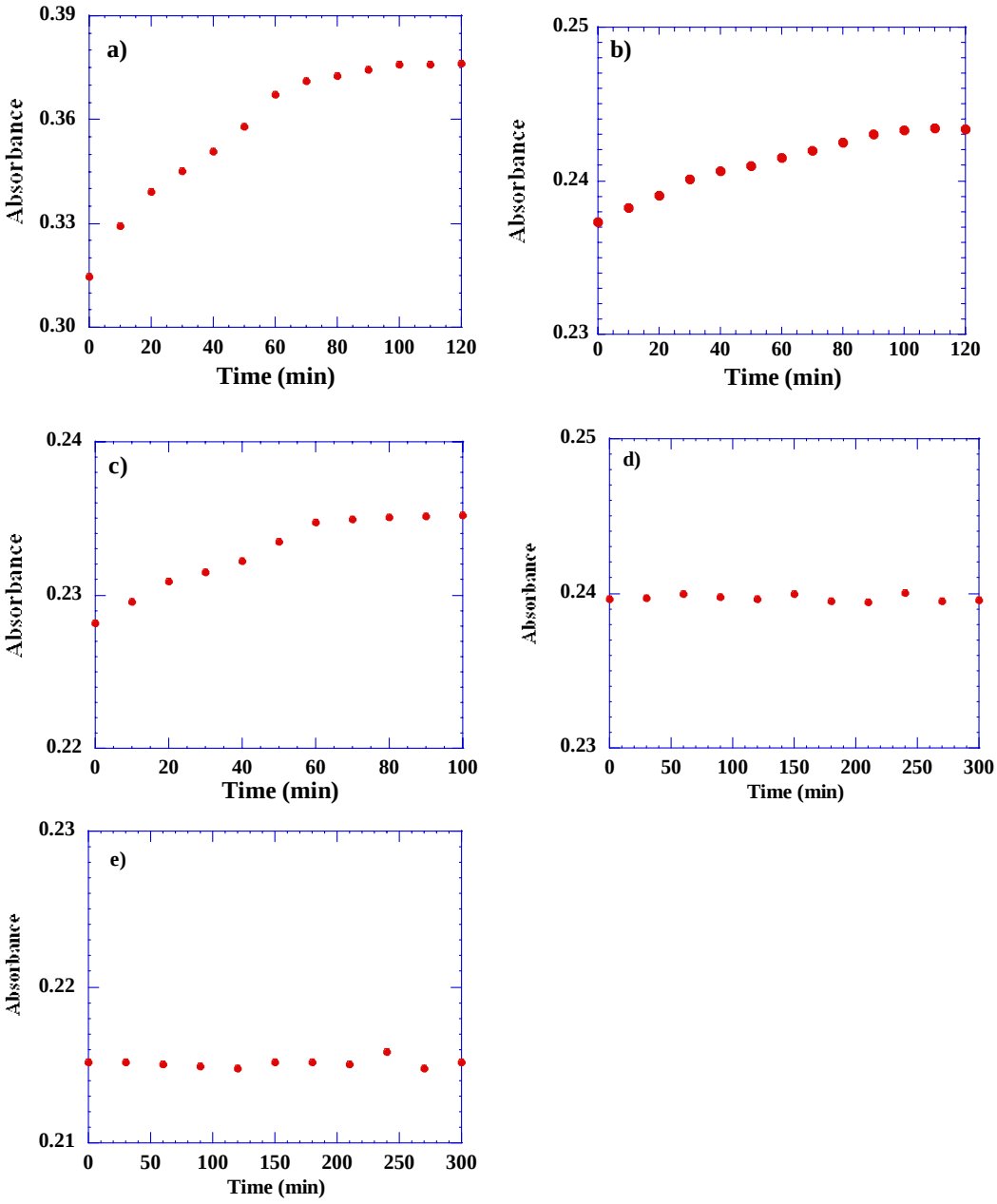


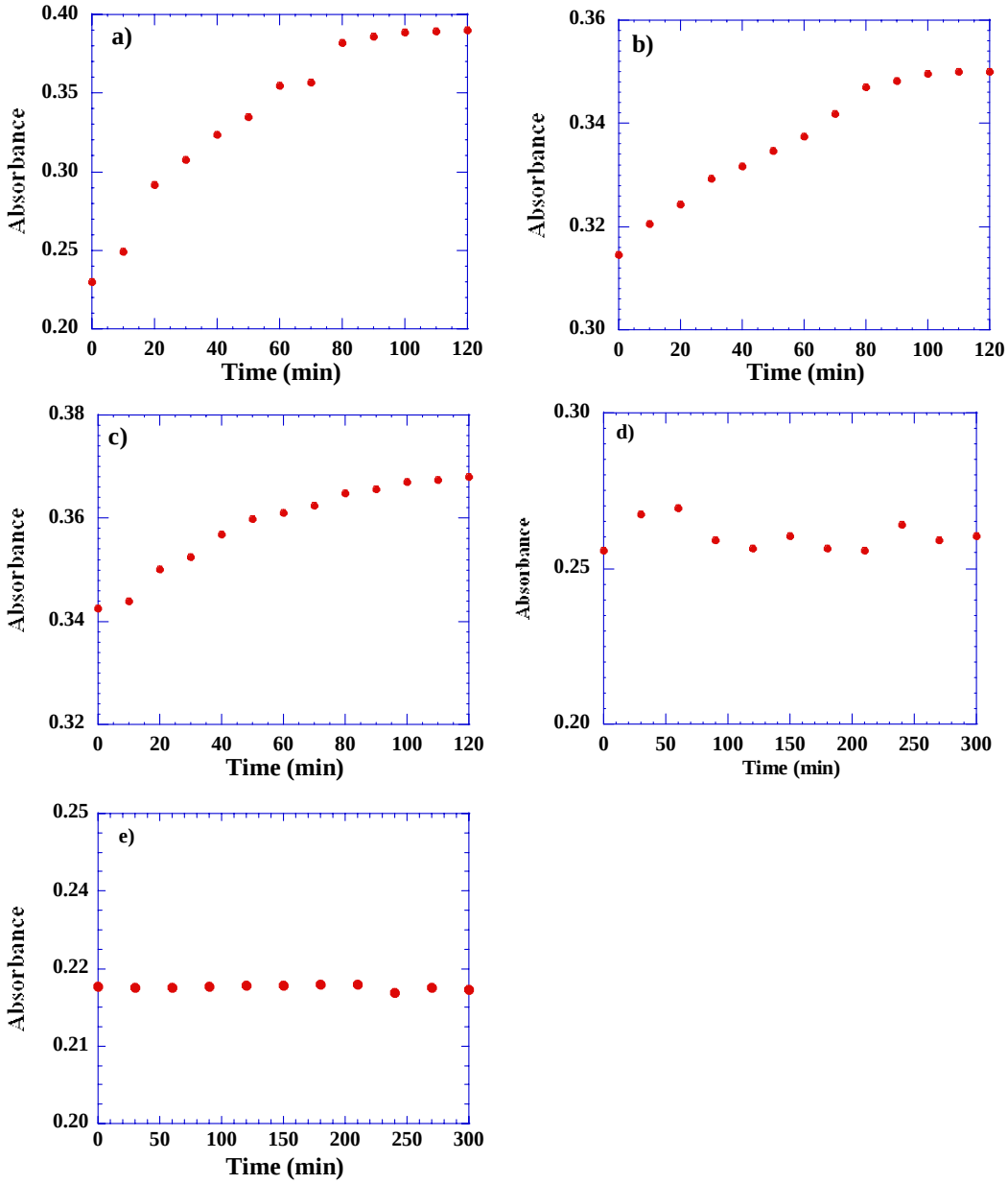
Fig. S5 Potential energy curves of interactions between the protonated **INH** and Qs. The infinite distance between the protonated **INH** and Qs has been considered as the null potential energy.

5. Kinetics plots of acetylation of INH in the absence and presence of Qs

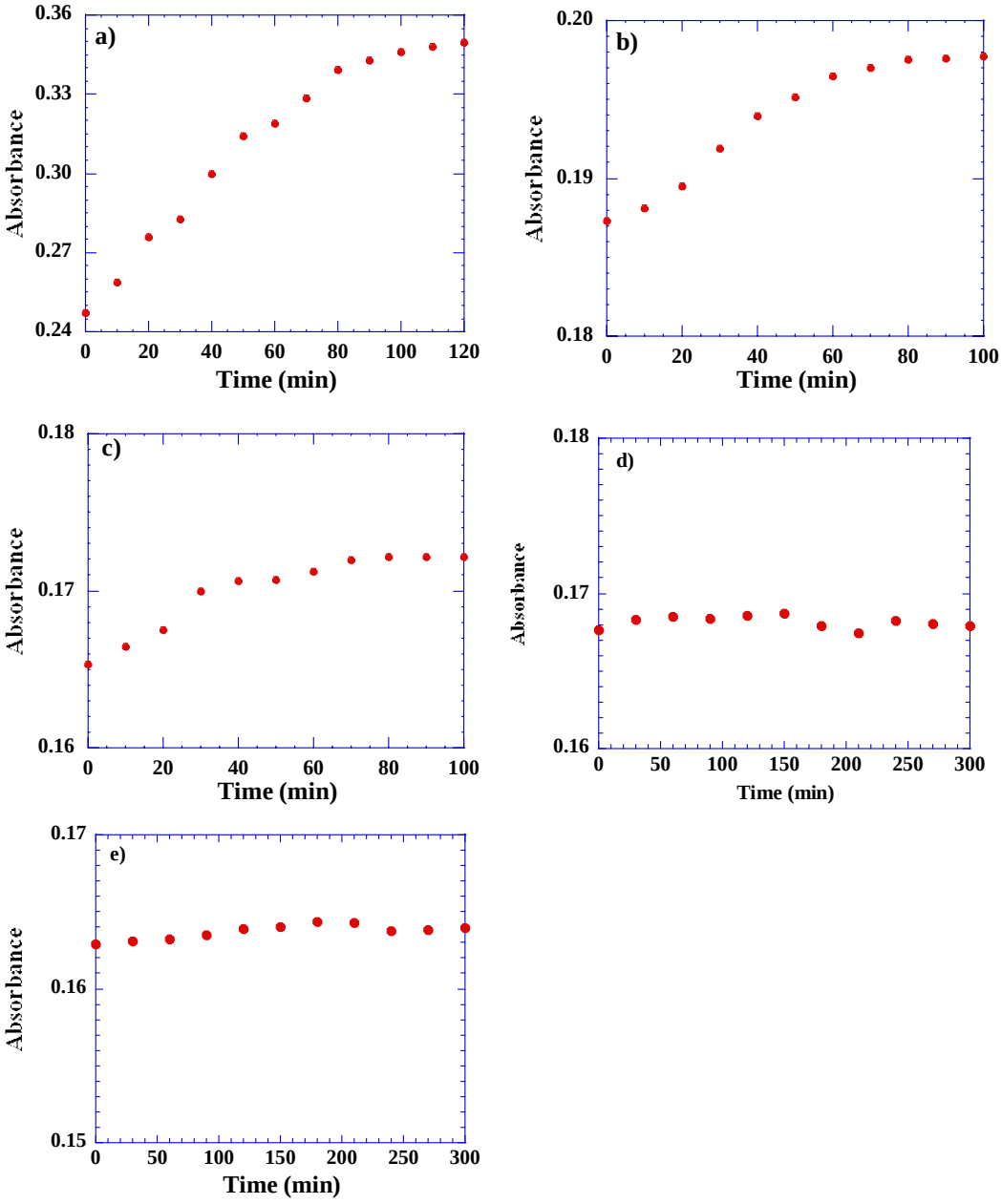
5.1. Kinetics plots of acetylation of **INH** with compound **1** a) in the absence of Qs, b) in the presence 0.8 eq. Q[6], c) in the presence 0.8 eq. Q[7], d) in the presence 1.0 eq. Q[6] and e) in the presence 1.0 eq. Q[7].



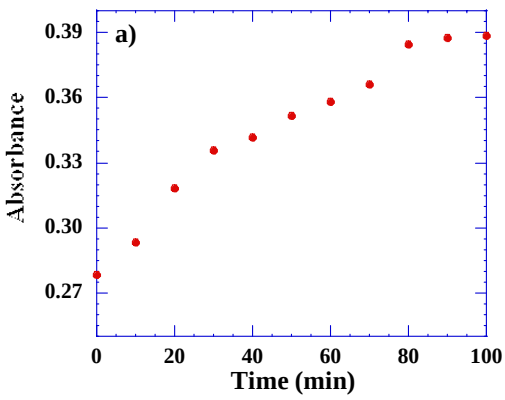
5.2. Kinetics plots of acylation of **INH** with compound **2** a) in the absence of Qs, b) in the presence 0.8 eq. Q[6], c) in the presence 0.8 eq. Q[7], d) in the presence 1.0 eq. Q[6] and e) in the presence 1.0 eq. Q[7].

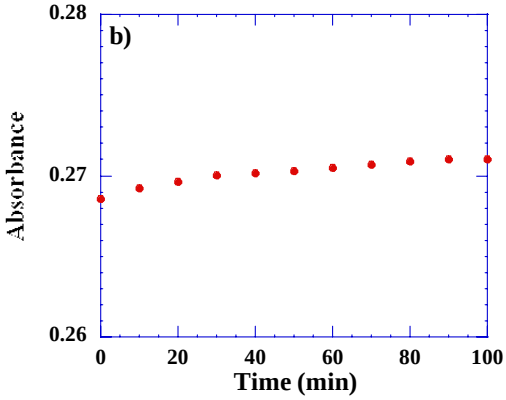


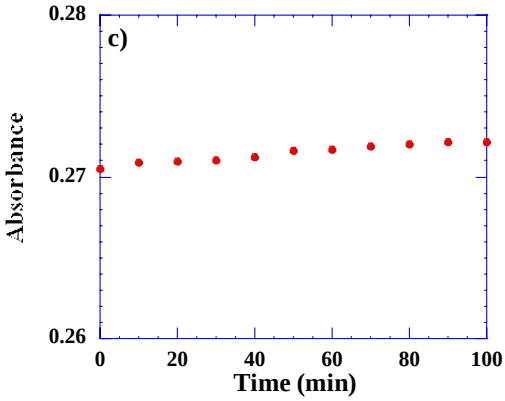
5.3. Kinetics plots of acylation of **INH** with compound **3** a) in the absence of Qs, b) in the presence 0.8 eq. Q[6] and c) in the presence 0.8 eq. Q[7].

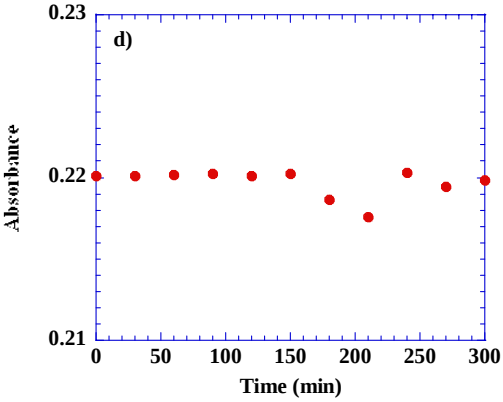


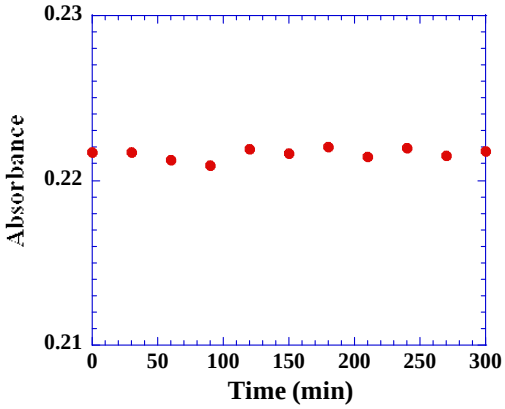
5.4. Kinetics plots of acylation of **INH** with compound **4** a) in the absence of Qs, b) in the presence 0.8 eq. Q[6], c) in the presence 0.8 eq. Q[7], d) in the presence 1.0 eq. Q[6] and e) in the presence 1.0 eq. Q[7].



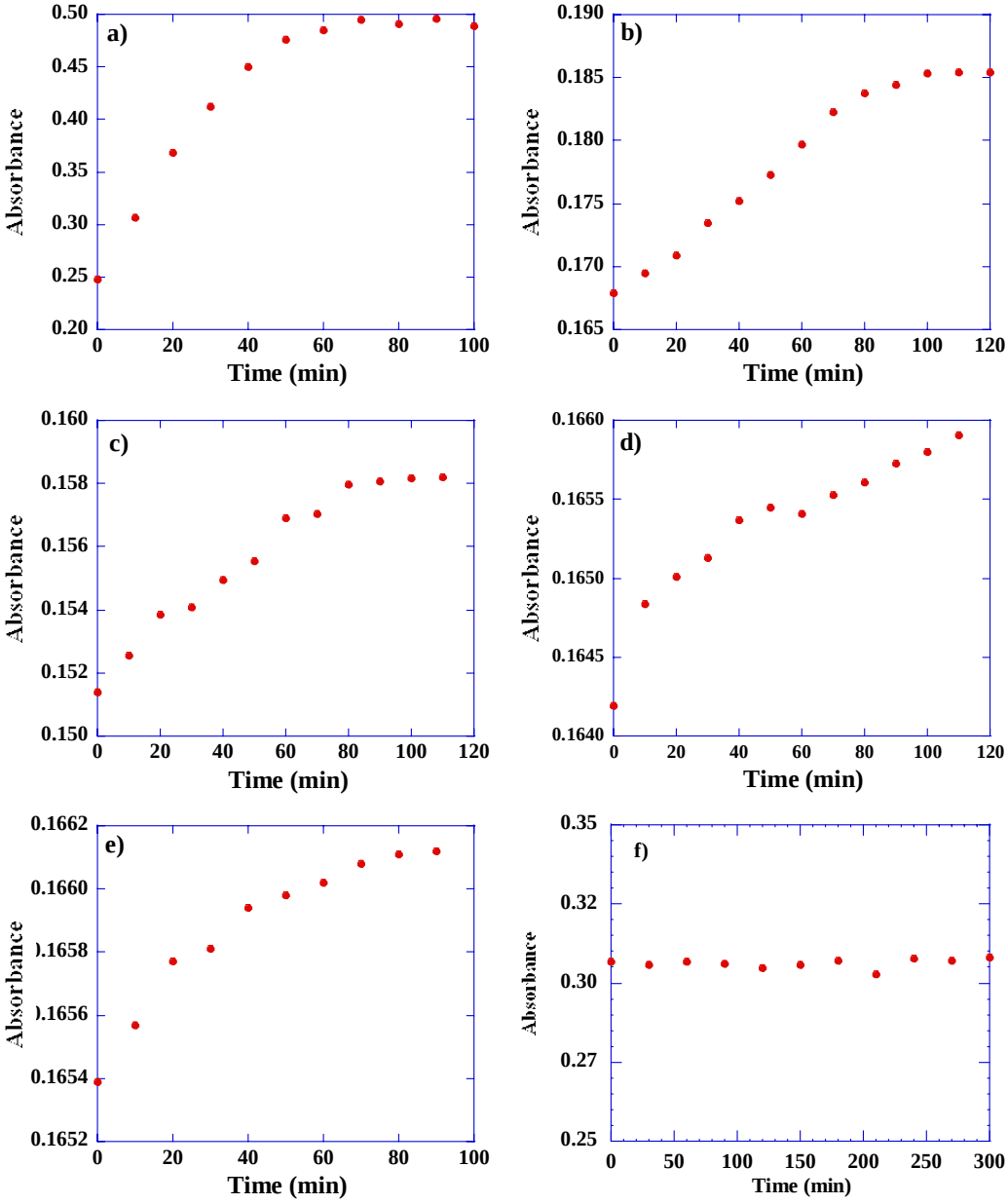




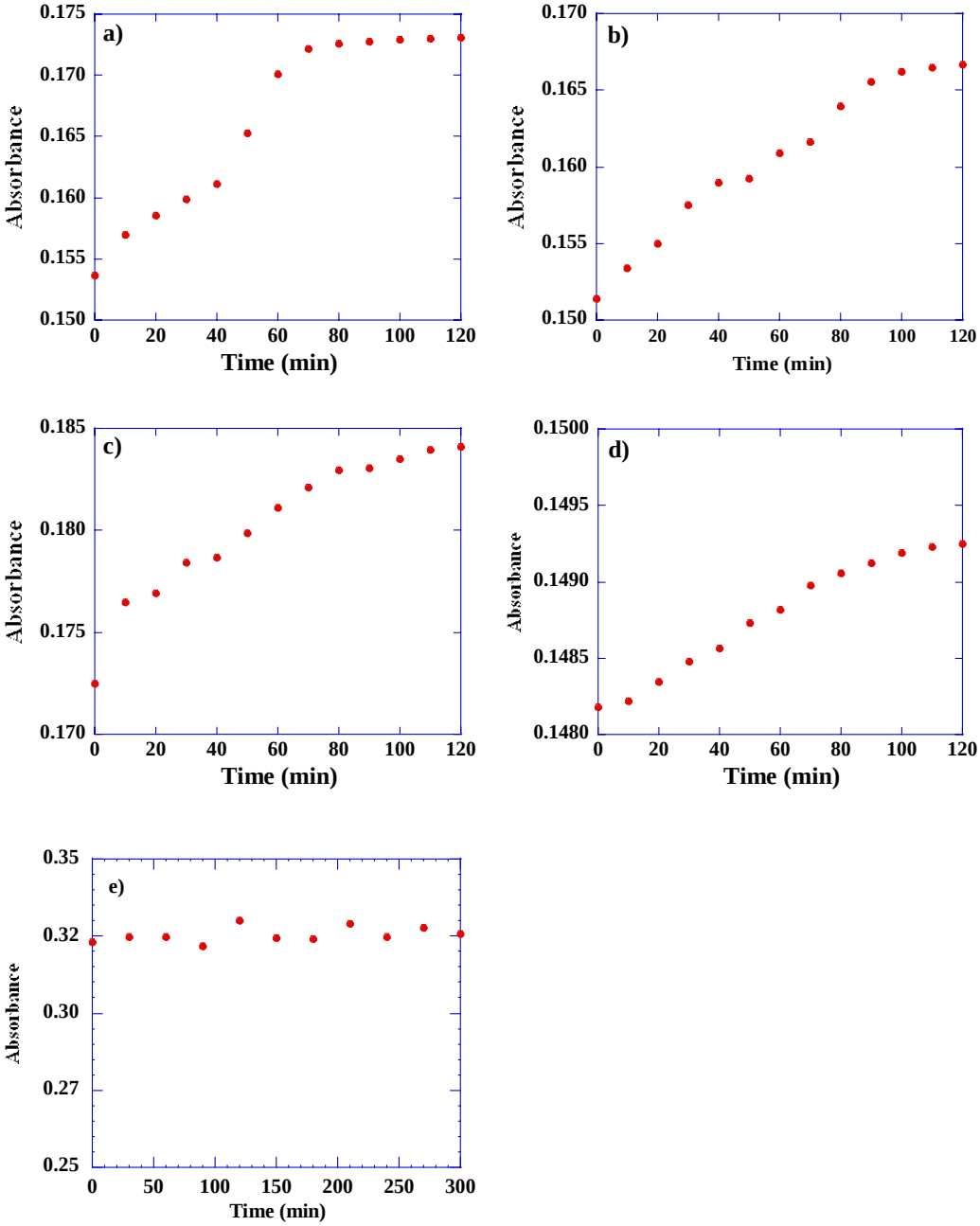




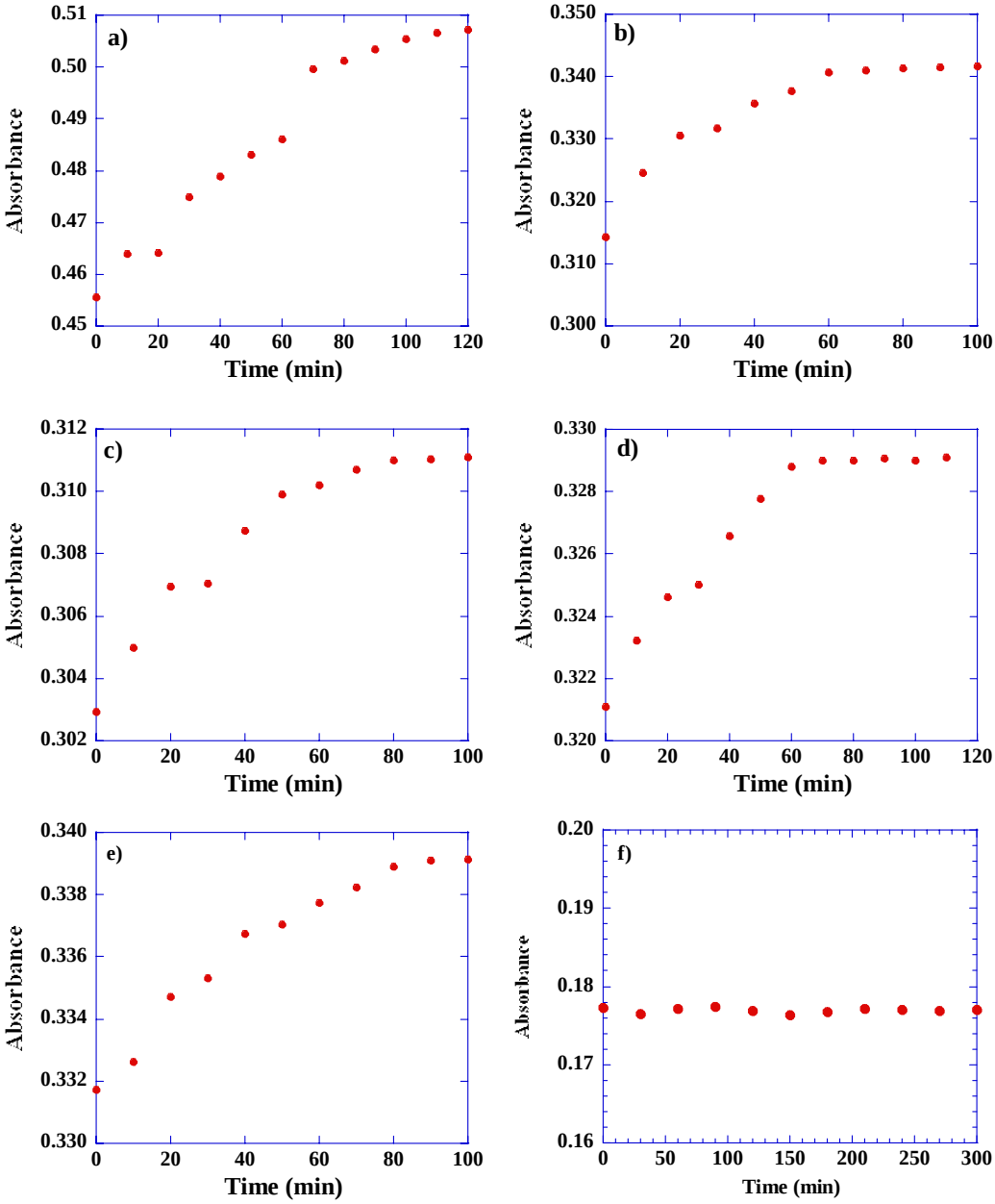
5.5. Kinetics plots of acylation of **INH** with compound **5** a) without Qs, and with Q[6] in a ratio of b) 0.2:1, c) 0.4:1, d) 0.6:1, e) 0.8:1, f) 1:1 ($C_{Q[6]}$:C_{INH}) at 40 °C.



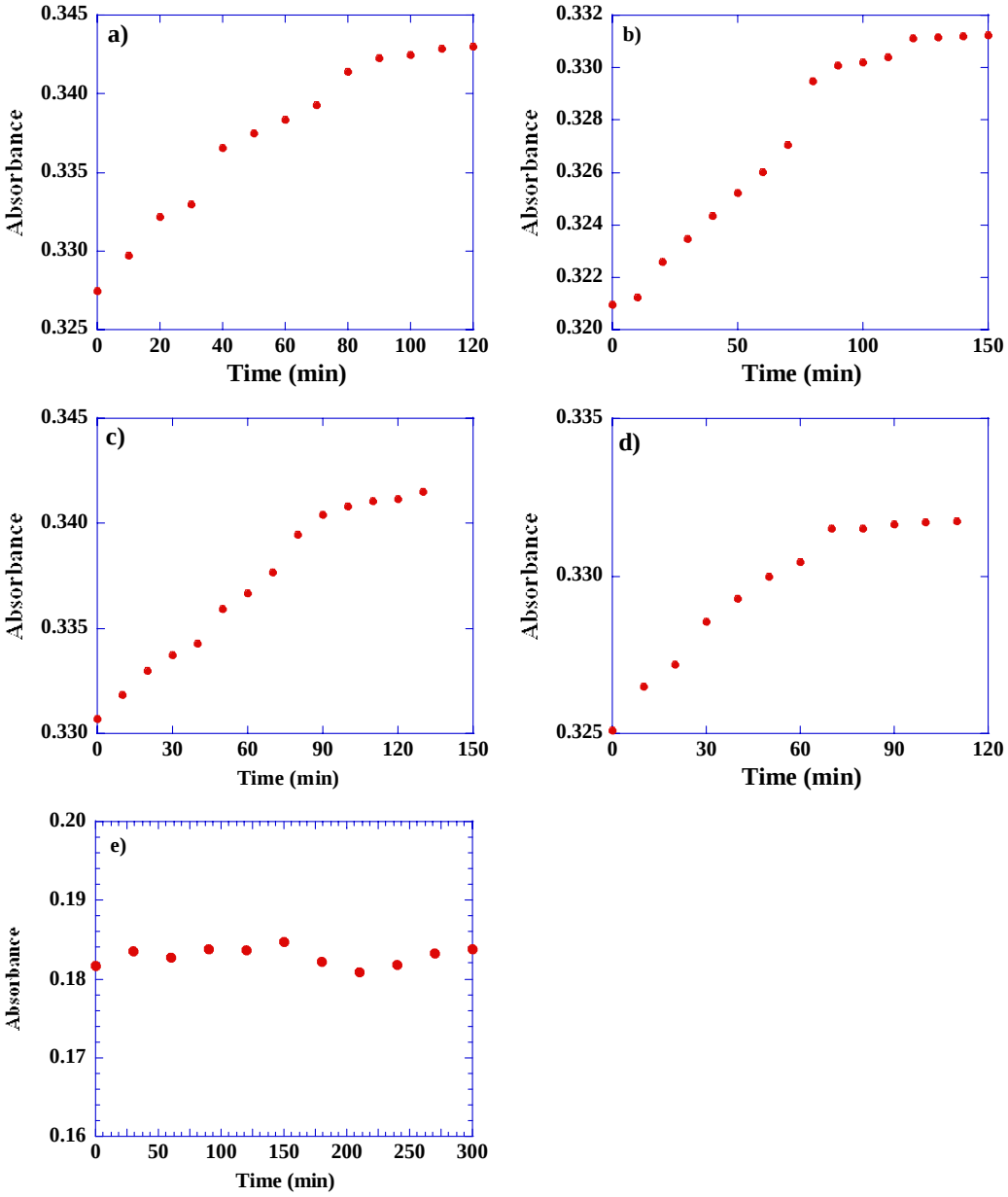
5.6. Kinetics plots of acylation of **INH** with compound **5** with Q[7] in a ratio of a) 0.2:1, b) 0.4:1, c) 0.6:1, d) 0.8:1, e) 1:1 ($C_{Q[7]}$:$C_{\mathbf{INH}}$) at 40 °C.



5.7. Kinetics plots of acylation of **INH** with compound **6** a) without Qs, and with Q[6] in a ratio of b) 0.2:1, c) 0.4:1, d) 0.6:1, e) 0.8:1, f) 1:1 ($C_{Q[6]}$:$C_{\mathbf{INH}}$) at 40 °C.



5.8. Kinetics plots of acylation of **INH** with compound **6** with Q[7] in a ratio of a) 0.2:1, b) 0.4:1, c) 0.6:1, d) 0.8:1, e) 1:1 ($C_{Q[7]}$:$C_{\mathbf{INH}}$) at 40 °C.



6. **Calculation of kinetics parameters**

The wavelength at 262 nm with the max absorbance of INH was tracked, and the initial rates (k) have been achieved by linear fitting of above kinetics plots in the first 50 minutes. The reaction hydrolysis of the acylating agents have been considered nearly similar for the fixed initial working concentration, so the kinetics parameters have been considered as observed initial rates (k_{obs}), which includes the background hydrolysis. Then pk_{obs} was calculated as following:

$$pk_{obs} = -\log(k_{obs})$$

The calculated values have been collected in **Table S1~2**

Table S1 Initial rates (pk_{obs}) of **INH** with acylating agents **1~4** in the absence and presence of Q [6 or 7]

Species of acylating agents	**1**	**2**	**3**	**4**
In the absence of Qs	2.94	2.55	2.78	2.73
In the presence of Q[6]	4.04	3.29	3.63	4.36
In the presence of Q[7]	3.83	3.36	3.79	4.62

Table S2 Initial reaction rates (pk_{obs}) of **INH** with thioester **5** and **6** in the presence of different mole ratio of Q[6 or 7] to **INH** at 40 °C.

Mole ratio of Qs to INH \ Different systems of Qs, INH and thioester	Q[6]-**INH**-**5**	Q[7]-**INH**-**5**	Q[6]-**INH**-**6**	Q[7]-**INH**-**6**
0.0	1.20	1.20	1.27	1.27
0.2	2.99	2.46	2.74	2.44
0.4	3.01	2.90	2.94	2.93
0.6	3.11	3.00	3.67	3.02
0.8	3.51	3.17	3.51	3.05
[a]1.0	***N***	***N***	***N***	***N***

[a] The addition of Q[6,7] in ratio of 1:1 to **INH** causes complete resistance to **INH** acetylation.

7. Coordinates of the optimized structures

(1) Q[6]@**INH**

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	0.0000	0.0000	0.0000
N	0.0000	1.3919	0.0000
C	1.2747	1.9508	0.0000
C	2.4882	1.2324	0.0194
C	2.4222	-0.1810	0.0319
C	1.1541	-0.8080	0.0065
C	3.6855	-1.0152	0.0261
N	4.8541	-0.5022	0.7039
N	5.8575	-1.6048	0.5446
O	3.8395	-2.1329	-0.6033
H	-0.9984	-0.4689	-0.0090
H	1.2930	3.0537	-0.0221
H	3.4741	1.7530	-0.0163
H	1.0729	-1.9039	-0.0028
H	4.6785	-0.0909	1.7251
H	6.7329	-1.2460	-0.0621
H	6.1644	-2.1343	1.4889
C	4.3629	1.1785	3.9520
C	4.6699	2.0922	6.1766
H	3.9958	2.2716	7.0477
C	4.7108	3.2856	5.1360
H	3.8250	3.9611	5.1943
C	6.8535	3.1834	6.2869
C	4.1321	3.3330	2.6156
H	3.3805	4.0548	3.0118
H	3.6305	2.5932	1.9583
C	6.4492	5.1955	4.7626
H	7.3688	5.5106	5.3043
C	5.5462	3.5274	0.5001
C	5.8955	5.2322	2.2353
C	6.8244	5.5573	0.9823
C	8.2324	5.2824	2.9735
C	6.9103	4.5001	-1.3962
H	6.0843	3.9775	-1.9276
H	6.9372	5.5773	-1.6713
C	9.4239	5.6860	0.7692
H	10.2484	5.8420	1.5009
H	9.3970	6.5102	0.0230
C	8.2638	-0.4884	7.1097

C	6.9324	-2.5380	7.0449
H	7.0695	-3.1989	7.9340
C	5.9731	-1.3012	7.3264
H	5.2957	-1.4525	8.2012
C	5.2046	-2.4631	5.3108
C	3.9404	-0.4020	5.9227
H	3.2977	-0.9577	5.2034
H	3.4275	-0.2876	6.9033
C	6.4976	1.2102	7.8216
H	7.3895	1.7447	8.2192
H	5.6712	1.2147	8.5671
N	4.1354	0.9668	5.3593
N	4.7225	2.5796	3.7880
N	6.1000	1.9596	6.5885
N	5.9451	4.0058	5.4972
N	5.0992	4.0595	1.7700
N	6.6410	4.3801	0.0743
N	6.8515	4.9510	3.3441
N	8.1765	5.7187	1.5827
N	8.1527	3.8400	-1.8708
N	6.9212	-0.1970	7.5971
N	6.2142	-3.2950	5.9716
N	5.1818	-1.2103	6.0509
O	4.2078	0.2830	3.0717
O	5.0588	2.5675	-0.1423
O	9.2630	0.2539	7.1353
O	7.9952	3.4767	6.6875
O	9.2278	5.2693	3.7223
O	4.4656	-2.7764	4.3559
C	12.3537	0.0350	1.3490
C	11.4395	-0.5732	-0.8495
H	12.0072	-0.8756	-1.7621
C	11.1976	-1.7734	0.1705
H	11.6759	-2.7327	-0.1423
C	9.0391	-0.9639	-0.6531
C	12.2334	-2.2413	2.4966
H	12.7216	-3.1151	2.0042
H	12.9704	-1.6754	3.1089
C	9.0445	-3.1022	0.8005
H	8.0069	-3.1610	0.4129
H	9.5999	-4.0232	0.5027
C	11.0825	-2.1855	4.7944
C	10.1281	-3.6625	3.1008
C	9.4547	-4.0055	4.5047

C	7.7234	-3.2237	2.9797
C	9.5117	-2.6482	6.7466
H	10.2631	-1.9625	7.1992
H	9.3671	-3.5499	7.3827
C	6.9016	-4.3118	5.1407
H	6.1132	-4.7464	4.4877
H	7.3427	-5.0967	5.7906
C	8.0874	2.4284	-2.2215
C	9.5136	4.2511	-1.4072
H	9.8141	5.1918	-1.9284
C	10.4400	3.0051	-1.7882
H	11.2311	3.2624	-2.5330
C	10.7703	3.5533	0.5756
C	12.3429	1.8467	-0.4396
H	12.9659	2.3001	0.3644
H	12.8545	1.9222	-1.4244
C	9.7824	0.5910	-2.5265
H	8.8678	0.1470	-2.9786
H	10.6629	0.4427	-3.1897
N	12.2214	0.4098	-0.0553
N	11.7412	-1.2911	1.4574
N	10.0574	-0.1524	-1.2452
N	9.7048	-1.9384	0.1620
N	11.2136	-2.7392	3.4500
N	10.1009	-3.0480	5.4430
N	8.9868	-3.0493	2.2997
N	7.9996	-3.8029	4.2508
N	8.2214	-1.8861	6.6437
N	9.4832	2.0282	-2.3896
N	9.6893	4.3917	0.0693
N	11.0524	2.5941	-0.4915
O	12.9383	0.6663	2.2487
O	11.7505	-1.2698	5.3082
O	7.0754	1.7451	-2.4726
O	7.7988	-0.8267	-0.8977
O	6.5470	-2.9473	2.5819
O	11.3354	3.6325	1.6834
H	5.6741	5.9947	4.8052
H	10.5145	-4.5571	2.5567
H	9.6264	-5.0584	4.8337
H	6.5303	6.4952	0.4524
H	5.2099	6.0713	2.5058
H	5.1355	-2.2356	-0.1067

total electronic energies: -4030.4616919 (a.u.) in gas
-4030.4626283 (a.u.) in water
BSSE-corrected energy: -4030.4114595 (a.u.)

(2) Q[7]@**INH**

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	0.0000	0.0000	0.0000
N	0.0000	1.3926	0.0000
C	1.2729	1.9616	0.0000
C	2.4794	1.2351	0.0362
C	2.4180	-0.1796	0.0407
C	1.1526	-0.8122	-0.0037
C	3.6316	-1.0560	0.1612
N	4.8894	-0.5807	0.5339
N	5.7563	-1.7824	0.6473
O	3.5622	-2.3768	0.0288
H	-0.9994	-0.4698	0.0118
H	1.2883	3.0680	-0.0324
H	3.4429	1.7617	0.0429
H	1.0882	-1.9209	-0.0270
H	5.3356	0.4824	0.5181
H	6.5687	-1.6782	-0.0235
H	6.0959	-1.8390	1.7133
C	-2.7990	-2.3366	3.1761
N	-1.7017	-3.2445	3.5464
N	-3.3232	-2.8444	1.9154
O	-3.2322	-1.3819	3.8498
C	-1.6203	-4.4073	2.6047
C	-2.4914	-3.9404	1.3577
C	-4.1838	-1.9761	1.0672
C	-1.4913	-3.4565	5.0143
N	-0.2812	-4.6413	2.0016
N	-1.4684	-3.5209	0.3364
N	-3.4618	-1.1704	0.0265
H	-1.9921	-5.3445	3.0839
H	-3.1422	-4.7484	0.9462
H	-4.6495	-1.2432	1.7643
H	-4.9622	-2.6094	0.5837
N	-0.1117	-3.2270	5.5064
H	-2.1271	-2.7003	5.5270
H	-1.8030	-4.4890	5.2983
C	-0.1289	-3.9576	0.7312
C	-3.4615	-1.6516	-1.3978

C	-1.8073	-3.6512	-1.1278
C	-3.6957	0.2834	0.0779
C	1.0352	-4.1027	5.1835
C	0.2782	-1.9719	6.1244
C	0.9085	-5.0790	2.7721
N	-2.2545	-2.4145	-1.8005
C	-3.3709	-0.3179	-2.2722
N	-3.3929	0.7744	-1.2559
H	-4.3830	-2.2479	-1.6054
O	0.9307	-3.7938	0.0831
O	-4.0681	0.9448	1.0667
H	-0.8743	-3.9494	-1.6555
H	-2.5888	-4.4380	-1.2437
N	1.6678	-2.1893	6.5201
C	2.2565	-3.4329	5.9650
O	-0.4320	-0.9822	6.3839
N	1.4742	-4.0879	3.7444
H	0.6500	-6.0210	3.3082
H	1.7110	-5.2618	2.0231
H	0.8263	-5.1512	5.5073
C	-1.3345	-1.6464	-2.6301
N	-2.1028	-0.4820	-3.0297
C	-3.8011	2.1675	-1.6031
H	-4.2247	-0.1994	-2.9837
N	3.2964	-3.2446	4.9122
C	2.8860	-3.7592	3.6089
H	2.6607	-4.0746	6.7853
C	2.4579	-1.1044	7.1245
N	-2.6992	3.1163	-1.8927
C	-1.5191	0.5610	-3.9030
O	-0.1953	-1.9845	-3.0093
H	-4.3158	2.5704	-0.7019
H	-4.4931	2.1435	-2.4758
O	3.6095	-3.8816	2.5986
C	4.7357	-3.1474	5.2332
N	3.3697	-0.3651	6.1708
H	3.0629	-1.5002	7.9728
H	1.7168	-0.3549	7.4844
C	-1.8197	3.0141	-3.0823
N	-0.9856	1.7704	-3.1984
C	-2.1246	3.9275	-0.8256
H	-0.6462	0.0839	-4.4031
H	-2.2802	0.8748	-4.6545
N	5.2909	-1.7496	5.2328

C	3.1669	1.0925	6.1180
C	4.8340	-0.6795	6.1740
H	4.9374	-3.5995	6.2292
H	5.3048	-3.6749	4.4352
C	0.4255	2.0822	-3.4022
C	-0.7420	4.1694	-2.8507
N	-1.0104	4.6118	-1.4633
H	-2.4237	3.1562	-4.0118
O	-2.5624	4.1054	0.3266
C	5.4951	0.6343	5.5739
C	5.8490	-1.2177	4.0268
N	4.4341	1.6466	5.6455
O	2.1374	1.7226	6.4203
H	5.1944	-0.9262	7.2021
N	0.5674	3.4892	-3.0538
C	-0.3067	5.7186	-0.8026
H	-0.8444	5.0220	-3.5667
O	1.3244	1.3120	-3.7977
N	5.8667	0.2137	4.1712
O	6.3372	-1.9342	3.0976
H	6.4114	0.9654	6.1206
C	4.7357	3.0949	5.7832
N	1.1224	5.4076	-0.4033
N	4.8922	3.8345	4.5058
H	-0.8548	5.9145	0.1464
H	-0.3151	6.6259	-1.4535
C	1.7946	4.2236	-3.4398
C	6.6722	1.1045	3.2939
H	5.6573	3.2258	6.3962
H	3.8594	3.5607	6.2881
C	2.2196	5.7872	-1.3703
N	2.6419	4.7207	-2.3125
C	1.4808	5.8560	0.9565
C	3.8101	4.6642	3.9899
C	5.9640	3.6102	3.5295
N	5.9039	2.2890	2.7655
H	2.4322	3.5056	-4.0024
H	1.5294	5.0970	-4.0788
H	7.5587	1.4907	3.8534
H	7.0182	0.4929	2.4341
N	2.8862	6.2586	0.8885
C	3.4861	5.9619	-0.4309
C	3.7643	3.9588	-1.8214
N	4.2512	5.0867	2.6585

C	5.8595	2.5385	1.3475
H	1.9546	6.7132	-1.9348
C	5.6676	4.7005	2.4082
H	6.9724	3.7077	3.9978
O	0.7306	5.9196	1.9483
O	2.7680	4.9958	4.5837
N	4.1762	4.6288	-0.5640
N	5.9008	3.9427	1.1350
C	3.6814	6.3752	2.1324
H	4.1637	6.7923	-0.7444
H	6.3561	5.5786	2.4402
O	5.8458	1.6973	0.3793
O	4.3325	2.9767	-2.3396
C	5.6182	4.5089	-0.2314
H	4.5002	7.1120	1.9733
H	2.9753	6.7328	2.9150
H	6.1426	5.4887	-0.2907
H	6.0498	3.7816	-0.9554
H	4.6933	-2.5326	0.2833

total electronic energies:-4624.3838038 (a.u.) in gas
-4624.3903157 (a.u.) in water
BSSE- corrected energy: -4624.3411171 (a.u.)

(3) Q[6]

Atomic Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	0.0000	0.0000	0.0000
N	0.0000	1.4512	0.0000
N	-1.4039	-0.3677	0.0000
O	0.9860	-0.7610	-0.0682
C	-1.3549	2.0575	-0.0282
C	-2.3336	0.7896	-0.0283
C	-1.8207	-1.7841	-0.1347
C	1.2647	2.2135	-0.1340
N	-1.7684	2.8160	1.1792
N	-3.1722	0.9970	1.1791
N	-2.2703	-2.4507	1.1111
N	1.7963	2.8156	1.1123
H	-1.4670	2.6984	-0.9381
H	-2.9821	0.7354	-0.9382
H	-0.9098	-2.3364	-0.4595
H	-2.6247	-1.8595	-0.9029
H	2.0296	1.4727	-0.4602

H	1.1335	3.0113	-0.9010
C	-2.8661	2.2120	1.9115
C	-3.6481	-2.3712	1.6586
C	-4.3401	0.1603	1.5453
C	-1.4089	-3.3881	1.8077
C	2.9190	2.2163	1.8097
C	1.3708	4.1273	1.6628
C	-1.2537	4.1571	1.5464
N	-4.0392	-1.0858	2.2904
C	-3.6242	-3.4006	2.8857
N	-2.2362	-3.9276	2.8710
N	3.2307	3.1503	2.8758
C	2.3710	4.3606	2.8920
N	0.0273	4.1801	2.2928
H	-4.3891	-2.6481	0.8677
H	1.4529	4.9161	0.8741
O	-3.4668	2.6755	2.9016
O	-0.2433	-3.7169	1.5089
O	3.5320	1.1722	1.5095
H	-4.9522	0.7835	2.2360
H	-4.9151	-0.0918	0.6244
H	-1.1541	4.7773	0.6259
H	-2.0119	4.5919	2.2366
C	-4.2747	-1.1754	3.7195
N	-4.0039	-2.5621	4.0507
C	-1.7474	-5.0319	3.7311
C	4.4207	2.9528	3.7378
N	1.4623	4.5137	4.0560
C	0.0525	4.4276	3.7225
H	-4.3525	-4.2414	2.7676
H	3.0014	5.2775	2.7773
N	-1.3090	-4.6488	5.0946
C	-4.2667	-3.0855	5.4128
C	1.9002	4.8978	5.4194
N	4.1571	2.4289	5.0996
O	-4.6951	-0.2796	4.4790
O	-0.9212	4.6081	4.4810
H	-0.8389	-5.4288	3.2237
H	-2.5350	-5.8171	3.8046
H	4.9826	3.9122	3.8152
H	5.0341	2.1745	3.2297
C	-2.2176	-4.4941	6.2586
N	-3.0761	-3.2829	6.2740
C	0.1008	-4.5622	5.4278

C	4.4281	1.0422	5.4306
C	3.7777	3.2672	6.2649
N	2.3897	3.7942	6.2800
H	-4.8797	-2.3070	5.9211
H	-4.8288	-4.0449	5.3362
H	0.9914	5.2943	5.9266
H	2.6873	5.6835	5.3457
C	-2.7645	-2.3493	7.3405
C	-1.2171	-4.2609	7.4875
N	0.1263	-4.3141	6.8573
N	4.1923	0.9522	6.8597
C	1.5625	3.2544	7.3433
H	-2.8488	-5.4103	6.3739
C	3.8018	2.2376	7.4918
H	4.5059	4.1080	6.3829
O	1.0744	-4.7428	4.6691
O	4.8487	0.1466	4.6710
N	-1.6421	-2.9490	8.0380
C	1.4074	-4.2907	7.6034
N	2.4242	2.3173	8.0399
C	4.4938	-0.2939	7.6045
H	-1.2993	-5.0496	8.2764
H	4.5431	2.5143	8.2824
O	0.3969	3.5829	7.6421
O	-3.3772	-1.3051	7.6407
N	1.9218	-2.9494	7.9703
N	3.3262	-1.1309	7.9710
C	1.9748	1.6502	9.2855
H	2.1655	-4.7254	6.9131
H	1.3083	-4.9108	8.5241
H	5.0691	-0.0418	8.5252
H	5.1058	-0.9169	6.9134
C	-1.1106	-2.3473	9.2846
C	1.5090	-2.1914	9.1784
N	0.1541	-1.5851	9.1512
C	3.0197	-2.3455	7.2382
C	2.4877	-0.9235	9.1785
N	1.5580	0.2338	9.1503
H	2.7790	1.7252	10.0535
H	1.0640	2.2023	9.6107
H	-1.8756	-1.6066	9.6110
H	-0.9796	-3.1454	10.0513
C	0.1541	-0.1339	9.1509
H	1.6216	-2.8327	10.0879

H	3.1362	-0.8694	10.0883
O	3.6201	-2.8089	6.2479
O	-0.8319	0.6272	9.2195

total electronic energies: -3563. 6519915 (a.u.) in gas
-3563.6519881 (a.u.) in water

(4) Q[7]

Atomic Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	0.0000	0.0000	0.0000
N	0.0000	1.4519	0.0000
N	-1.4043	-0.3684	0.0000
O	0.9865	-0.7612	-0.0592
C	-1.3546	2.0553	-0.0719
C	-2.3318	0.7886	-0.0724
C	-1.8230	-1.7751	-0.2103
C	1.2547	2.2137	-0.2089
N	-1.7884	2.8312	1.1173
N	-3.1931	1.0112	1.1162
N	-2.4052	-2.4539	0.9724
H	-1.4457	2.6835	-0.9932
H	-2.9619	0.7175	-0.9942
H	-0.8932	-2.3363	-0.4568
H	-2.5486	-1.8217	-1.0568
N	1.7627	2.9495	0.9738
H	2.0335	1.4564	-0.4542
H	1.1171	2.9269	-1.0561
C	-2.9174	2.2500	1.8213
C	-3.8268	-2.3264	1.3814
C	-4.4154	0.2241	1.4078
C	-1.6913	-3.5245	1.6448
C	1.2779	4.2924	1.3813
C	2.9812	2.5334	1.6448
C	-1.3382	4.2132	1.4097
N	-4.1941	-1.0740	2.0892
C	-3.9992	-3.4561	2.5010
N	-2.6530	-4.0769	2.5816
H	-4.4949	-2.4764	0.4966
O	-3.5540	2.7406	2.7753
O	-0.5320	-3.9256	1.4182
H	-5.0140	0.8416	2.1152
H	-4.9785	0.0521	0.4598
N	3.2711	3.6052	2.5802

C	2.3274	4.7486	2.4990
O	3.6648	1.5148	1.4185
N	-0.0261	4.3297	2.0903
H	-1.3160	4.8027	0.4624
H	-2.0873	4.6342	2.1181
H	1.2515	4.9750	0.4953
C	-4.6096	-1.2741	3.4659
N	-4.4425	-2.6975	3.6978
C	-2.3665	-5.3315	3.3180
H	-4.7622	-4.2296	2.2337
N	1.4824	4.9855	3.6965
C	0.0632	4.7847	3.4663
H	2.8807	5.6831	2.2301
C	4.5580	3.6488	3.3154
N	-2.1358	-5.1815	4.7750
C	-4.9564	-3.3346	4.9341
O	-5.0731	-0.4238	4.2521
H	-1.4124	-5.7217	2.8967
H	-3.1983	-6.0560	3.1494
O	-0.8763	5.0179	4.2531
C	1.9689	5.6464	4.9315
N	4.4734	3.3892	4.7727
H	5.0470	4.6371	3.1446
H	5.1775	2.8246	2.8946
C	-3.2259	-5.1068	5.7802
N	-3.9250	-3.8017	5.8914
C	-0.8179	-5.3890	5.3478
H	-5.5324	-2.5449	5.4676
H	-5.6189	-4.1897	4.6600
N	2.6843	4.7693	5.8893
C	5.0103	2.1684	5.3464
C	4.1243	4.4254	5.7772
H	2.6262	6.5049	4.6559
H	1.0588	6.0022	5.4655
C	-3.7363	-3.1381	7.1689
C	-2.4597	-5.2440	7.1777
N	-1.0346	-5.3790	6.7834
H	-3.9680	-5.9248	5.6018
O	0.2515	-5.5987	4.7409
C	4.4535	3.7210	7.1752
C	2.0918	4.4195	7.1678
N	4.9466	2.3769	6.7818
O	5.4851	1.1869	4.7402
H	4.7259	5.3513	5.5966

N	-2.8237	-3.9988	7.8998
C	0.0475	-5.7659	7.7204
H	-2.7792	-6.1376	7.7703
O	-4.2895	-2.0963	7.5745
N	3.1572	3.7569	7.8984
O	0.9439	4.6897	7.5743
H	5.2368	4.2582	7.7665
C	5.5968	1.4300	7.7193
N	0.6110	-4.6655	8.5389
N	4.6764	0.6054	8.5386
H	0.8849	-6.1322	7.0842
H	-0.3201	-6.5760	8.3941
C	-2.5436	-3.7669	9.3373
C	3.0056	3.4283	9.3363
H	6.2863	1.9926	8.3925
H	6.1646	0.7131	7.0838
C	-0.0008	-4.1787	9.8010
N	-1.1776	-3.2855	9.6549
C	1.9622	-4.1844	8.3142
C	4.5541	-0.8237	8.3138
C	4.0501	1.0736	9.8007
N	2.8872	1.9851	9.6548
H	-3.2349	-2.9538	9.6551
H	-2.7468	-4.7038	9.9085
H	3.8610	3.8629	9.9060
H	2.0441	3.8908	9.6551
N	2.2258	-3.2923	9.4289
C	1.1229	-3.2232	10.4204
C	-0.9556	-1.9335	10.1351
N	3.7580	-1.3051	9.4285
C	1.6360	1.4269	10.1352
H	-0.2573	-5.0449	10.4611
C	3.4113	-0.2560	10.4202
H	4.8227	1.5413	10.4610
O	2.7476	-4.5179	7.4042
O	5.0763	-1.4987	7.4040
N	0.4370	-1.9124	10.5453
N	1.9694	0.0747	10.5456
C	3.5874	-2.7578	9.6714
H	1.4871	-3.5618	11.4226
H	3.8315	-0.5226	11.4223
O	0.5349	2.0039	10.2385
O	-1.7933	-1.0150	10.2382
C	0.9943	-0.7578	11.2902

H	3.8967	-2.9962	10.7168
H	4.2508	-3.2696	8.9379
H	1.4640	-1.1202	12.2354
H	0.1298	-0.0912	11.5104

total electronic energies: -4157.5974559 (a.u.) in gas
-4157.597456 (a.u.) in water

(5) **INH**

Atomic Symbol	Coordinates (Angstroms)		
	X	Y	Z
C	0.0000	0.0000	0.0000
N	0.0000	1.3950	0.0000
C	1.2724	1.9703	0.0000
C	2.4847	1.2536	-0.0062
C	2.4275	-0.1669	-0.0092
C	1.1570	-0.8055	-0.0023
C	3.6462	-1.0159	-0.0103
N	4.9706	-0.4986	-0.0768
N	5.8880	-1.6513	-0.1891
O	3.6233	-2.3373	0.1108
H	-0.9991	-0.4702	0.0030
H	1.2868	3.0742	0.0066
H	3.4393	1.7978	0.0084
H	1.0833	-1.9036	-0.0011
H	5.2076	0.4074	-0.5574
H	6.6150	-1.5815	0.5806
H	4.7396	-2.4878	-0.0004
H	6.3871	-1.6374	-1.1263

total electronic energies: -466. 2120888 (a.u.) in gas
-466.2121576 (a.u.) in water