Supporting Information: Linear-response time-dependent embedded mean-field theory

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Cartesian coordinates for the test molecules

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Decanoic acid

O	-4.948361	1.342597	-0.000731
O	-5.890651	-0.729041	-0.017629
H	-6.682665	-0.161116	-0.022450
C	-4.815839	0.128576	-0.004071
H	-3.516974	-1.294029	0.895855
H	-3.510364	-1.312853	-0.866177
C	-3.507328	-0.638128	0.007669
H	-2.304362	0.925329	-0.884875
H	-2.307476	0.938863	0.880661
C	-2.272305	0.271464	0.003068
H	-0.937369	-1.189510	0.901278
H	-0.934245	-1.200899	-0.870891
C	-0.961911	-0.533552	0.010908
H	0.262641	1.019182	-0.881438
H	0.263463	1.026113	0.890356
C	0.288978	0.361359	0.007053
H	1.629362	-1.095061	0.898012
H	1.627247	-1.102598	-0.874041
C	1.603676	-0.437174	0.009210
H	2.828592	1.116513	-0.883144

H	2.834599	1.119274	0.888699
C	2.855989	0.456134	0.003736
H	4.198052	-1.003686	0.887474
H	4.191324	-1.006812	-0.884571
C	4.170123	-0.343095	0.000376
H	5.393340	1.208888	-0.891433
H	5.401533	1.210074	0.878865
C	5.422997	0.548684	-0.005949
H	7.612748	0.396879	-0.015292
H	6.785709	-0.909114	-0.902400
H	6.793434	-0.909042	0.879056
C	6.729537	-0.261741	-0.011445

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Nonylbenzene

H	3.854360	-2.159819	0.316410
C	4.326698	-1.207800	0.082103
C	5.558232	-1.190668	-0.574661
H	6.037391	-2.127281	-0.848545
C	6.176048	0.025378	-0.873490
H	7.136697	0.041250	-1.381441
C	5.552981	1.220840	-0.509319
H	6.028083	2.172909	-0.732295
C	4.321579	1.197226	0.147337
H	3.845274	2.133195	0.432755
C	3.688349	-0.015846	0.452242
C	2.333179	-0.036750	1.127250
H	2.243126	-0.939059	1.746954
H	2.247703	0.819182	1.810328
C	1.158974	0.002333	0.127557
H	1.247136	0.905155	-0.492987
H	1.247037	-0.849330	-0.561508
C	-0.214968	-0.024742	0.808928
H	-0.294890	-0.929387	1.430142
H	-0.294233	0.826318	1.501833
C	-1.387889	0.015888	-0.179966
H	-1.309544	0.922271	-0.798526
H	-1.305954	-0.833033	-0.874904
C	-2.763317	-0.017026	0.499612
H	-2.841175	-0.924050	1.117504
H	-2.844726	0.831280	1.195539
C	-3.936955	0.024315	-0.488265
H	-3.860145	0.932209	-1.105032
H	-3.854423	-0.823016	-1.185283
C	-5.312273	-0.011636	0.190898

H	-5.389740	-0.919538	0.807819
H	-5.396097	0.835731	0.887912
C	-6.486458	0.029034	-0.796211
H	-6.409850	0.936324	-1.412379
H	-6.403449	-0.818053	-1.492166
C	-7.855969	-0.007505	-0.109665
H	-7.976068	-0.920347	0.487000
H	-7.984005	0.847354	0.565986
H	-8.671775	0.021489	-0.841209

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Decapentaene

C	-3.96500000	-1.04260000	0.00000000
H	-4.55860000	-0.11860000	0.00000000
H	-4.55860000	-1.96660000	0.00000000
C	-2.63910000	-1.04260000	0.00000000
H	-2.04550000	-1.96670000	0.00000000
C	-1.80670000	0.25300000	0.00000000
H	-2.40030000	1.17710000	0.00010000
C	-0.48080000	0.25300000	0.00000000
H	0.11280000	-0.67100000	0.00000000
C	0.35160000	1.54870000	0.00010000
H	-0.24200000	2.47270000	0.00020000
C	1.67750000	1.54860000	0.00010000
H	2.27110000	0.62460000	0.00000000
C	2.50990000	2.84430000	0.00020000
H	1.91630000	3.76830000	0.00030000
C	3.83580000	2.84420000	0.00020000
H	4.42940000	1.92020000	0.00010000
C	4.66820000	4.13990000	0.00030000
H	4.07460000	5.06390000	0.00040000
C	5.99410000	4.13990000	0.00030000
H	6.58770000	5.06390000	0.00040000
H	6.58770000	3.21580000	0.00020000

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Chlorophyll a

Mg	6.6190510	-3.9832090	1.2235690
N	7.2575730	-5.0737070	2.7953720
N	5.9828680	-2.8530730	-0.3385310
N	6.7622710	-2.3119020	2.4426630
N	6.4971580	-5.7741450	0.0423210
C	7.4221660	-6.3981010	2.7317310
C	6.7561810	-7.0642910	0.4475750
C	6.1804320	-5.7506240	-1.2777260
C	5.6870250	-3.2944970	-1.5943740

C	5.7693570	-1.4904340	-0.3148600
C	6.4548250	-1.0355690	2.0685120
C	7.1845660	-2.2573010	3.7539560
C	7.6357860	-4.6998990	4.0842530
C	7.2036370	-7.3610950	1.7202120
C	5.7986020	-4.6359630	-2.0160430
C	5.9905720	-0.6694670	0.7865520
C	7.5888310	-3.3683730	4.5113280
C	7.9093650	-6.9303350	3.9556020
C	7.5666330	-8.7132080	2.3308400
C	8.0548170	-5.8652470	4.8387700
C	8.0661890	-8.3725430	3.8145860
C	5.3130390	-1.0533100	-1.6319150
C	5.2577380	-2.1840950	-2.4259240
C	6.6825730	-0.1216690	3.1711440
C	7.1394920	-0.8837800	4.2249100
C	6.4734650	-8.0578650	-0.6709300
C	6.3344640	-7.1319210	-1.9079610
O	8.4711510	-9.2044280	4.6023300
C	4.9650120	0.3253290	-1.9606550
C	5.0420160	0.9116940	-3.1657510
H	4.6121650	0.9321970	-1.1271540
H	5.4248320	0.3995830	-4.0426650
H	4.7425800	1.9470760	-3.3003900
C	8.6517940	-9.4804440	1.5939030
C	5.2024880	-8.8921550	-0.3876480
C	3.7472790	-10.8459340	-1.1504690
O	9.4582980	-9.0011830	0.8233980
O	2.6359070	-10.0785910	-1.1419780
C	4.9842450	-10.0099620	-1.4246810
C	8.5397450	-5.9015760	6.2550410
O	8.6173290	-10.7838640	1.9293110
C	4.8017340	-2.2962350	-3.8488510
O	3.7528930	-12.0437450	-0.9557620
C	7.5592640	-0.4148700	5.5910340
C	6.4586510	1.3613030	3.1235410
C	7.5560500	-7.1918420	-2.8437550
C	9.6656640	-11.5940110	1.3750710
C	9.0765780	-0.1724880	5.7152960
C	1.3679240	-10.7713170	-0.9293390
C	0.8093800	-11.2884310	-2.2199420
C	0.5894050	-12.5713130	-2.5542610
C	-0.0042220	-12.9096160	-3.9087030
C	0.9737440	-13.6085190	-4.8826030
C	2.1995050	-12.7560320	-5.2382880
C	3.1098180	-13.3436350	-6.3375340

C	4.1484090	-12.2862720	-6.7748070
C	5.0572440	-12.6792000	-7.9654030
C	6.4609890	-13.1583880	-7.5596500
C	0.8743950	-13.7455480	-1.6459010
C	3.7601230	-14.6647290	-5.8980180
C	7.3375060	-13.6823520	-8.7167120
C	7.5801250	-12.6541850	-9.8486100
C	8.3031140	-11.3605020	-9.4404060
C	8.4547570	-10.3369430	-10.5811920
C	9.3092790	-10.7656600	-11.7928800
C	10.7568540	-11.0998380	-11.4014220
C	8.6572610	-14.2537150	-8.1704830
C	9.2819120	-9.6718000	-12.8718500
H	6.7081610	-9.3848470	2.4527980
H	7.8965630	-3.1736810	5.5346740
H	5.8005810	0.3892640	0.6419000
H	5.5691380	-4.8262880	-3.0600550
H	7.3248030	-8.7384880	-0.7881690
H	9.4405550	-5.2887450	6.3884180
H	7.7833130	-5.5174320	6.9515440
H	8.7805950	-6.9274470	6.5451310
H	5.4371810	-7.3771660	-2.4899780
H	5.6338440	-2.2003780	-4.5605050
H	4.3219810	-3.2618380	-4.0412540
H	4.0797900	-1.5086140	-4.0885730
H	6.5944370	1.8185100	4.1082250
H	7.1566950	1.8566710	2.4354670
H	5.4445350	1.6077800	2.7841440
H	7.0287080	0.5125080	5.8387960
H	7.2482460	-1.1460040	6.3483830
H	5.2771210	-9.3445300	0.6082550
H	4.3272570	-8.2326000	-0.3679650
H	8.4780130	-6.9731340	-2.2933020
H	7.6542000	-8.1910260	-3.2840220
H	7.4666840	-6.4663070	-3.6594220
H	4.8818860	-9.5755860	-2.4274350
H	5.8369090	-10.6949920	-1.4398200
H	1.5161570	-11.5536760	-0.1851730
H	0.7258250	-9.9920870	-0.5082080
H	10.6431180	-11.2307070	1.7029780
H	9.4851500	-12.6011180	1.7513410
H	9.6278400	-11.5780370	0.2822550
H	9.6410210	-1.0874880	5.5044930
H	9.4091240	0.5918410	5.0043950
H	9.3367060	0.1642600	6.7256320
H	0.5605420	-10.5138370	-2.9454740

H -0.8740940 -13.5678100 -3.7640330
H -0.3792500 -11.9932350 -4.3819840
H -0.0445410 -14.0786910 -1.1429930
H 1.2411230 -14.6018120 -2.2231090
H 1.6278280 -13.5168170 -0.8900060
H 1.2893410 -14.5690720 -4.4574790
H 0.4193510 -13.8511980 -5.8002930
H 1.8481600 -11.7666100 -5.5680540
H 2.7961370 -12.5777030 -4.3327090
H 2.4776710 -13.5574650 -7.2151400
H 3.5961130 -11.3729050 -7.0334920
H 4.7739510 -12.0201770 -5.9090690
H 3.0080850 -15.4150910 -5.6311140
H 4.3748680 -15.0958830 -6.6952040
H 4.4038220 -14.5121190 -5.0216010
H 4.5622500 -13.4577070 -8.5649710
H 5.1590600 -11.8141360 -8.6323670
H 6.9805770 -12.3374940 -7.0439450
H 6.3702520 -13.9598220 -6.8147490
H 6.7901430 -14.5191450 -9.1790750
H 8.1547510 -13.1586980 -10.6375950
H 6.6175260 -12.3885790 -10.3076560
H 9.2378970 -13.4918120 -7.6365710
H 9.2864680 -14.6464420 -8.9788310
H 8.4683960 -15.0731460 -7.4666990
H 7.7464170 -10.8737090 -8.6284590
H 9.2901010 -11.5974830 -9.0236720
H 7.4522320 -10.0645140 -10.9435200
H 8.8867990 -9.4133280 -10.1665870
H 8.8605780 -11.6696520 -12.2301260
H 11.3483500 -11.3707550 -12.2842420
H 11.2433770 -10.2360230 -10.9287230
H 10.8111520 -11.9382630 -10.6984760
H 9.7259560 -8.7399280 -12.4972310
H 9.8484100 -9.9749070 -13.7606520
H 8.2559890 -9.4469850 -13.1880400

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pNA in 18 H2O
C -1.90522 -0.01966 -0.22680
C -1.03688 -1.16033 -0.28773
C 0.32133 -1.01155 -0.26866
C 0.88623 0.29164 -0.24882
C 0.04313 1.43027 -0.28896
C -1.31357 1.28810 -0.27757
N 2.25503 0.44338 -0.12039

O	3.00963	-0.56036	-0.04718
O	2.76737	1.60889	-0.06841
H	-1.47062	-2.15427	-0.25046
H	0.97795	-1.87171	-0.22918
H	0.47040	2.42065	-0.32071
H	-1.95046	2.16600	-0.29343
N	-3.21488	-0.15377	-0.09125
H	-3.64098	-1.07206	-0.16166
H	-3.81235	0.69161	0.00527
H	4.91221	-0.94953	-2.87434
O	5.04531	-1.53612	-2.11484
H	5.50991	-0.94836	-1.48785
H	4.57986	1.23177	-0.84920
O	5.45890	1.04888	-1.22805
H	6.03674	1.72336	-0.84195
H	2.17691	3.40834	0.38857
O	1.70513	4.24911	0.55200
H	2.42584	4.83534	0.84037
H	-2.03765	4.57802	-0.41440
O	-2.68480	4.27889	0.25878
H	-2.12597	4.20293	1.06459
H	-4.98130	2.21685	-0.73797
O	-4.58800	2.25026	0.14985
H	-3.97102	3.02311	0.14477
H	-4.57597	-1.08274	1.97061
O	-4.50389	-2.04551	1.90151
H	-3.54424	-2.23320	2.04565
H	-4.48155	-3.38726	-1.47605
O	-4.52593	-2.45557	-1.74077
H	-4.21807	-2.42631	-2.65922
H	0.16595	-3.75922	-1.89457
O	0.58682	-4.31957	-1.22606
H	1.53252	-4.05415	-1.26632
H	3.94034	-3.72235	-1.49422
O	3.16135	-3.23652	-1.17515
H	3.49150	-2.31243	-1.28784
H	-6.00654	-1.74628	-0.68277
O	-6.54638	-1.41041	0.04987
H	-6.20068	-1.93065	0.79767
H	4.85916	-1.05719	0.78390
O	5.44191	-1.78541	1.04683
H	4.83872	-2.41641	1.47270
H	-0.21865	4.15661	-2.02707
O	-0.38474	4.81963	-1.34154
H	0.39347	4.76871	-0.74949
H	-0.67550	2.90062	2.28552

O	-0.65437	3.86399	2.18152
H	0.18705	4.04038	1.71023
H	0.04078	-4.31791	0.53384
O	0.00315	-4.04152	1.47461
H	0.93086	-3.78642	1.66108
H	5.11569	3.61336	1.79058
O	4.51143	3.58331	1.03389
H	4.22890	2.65664	0.97915
H	-1.19044	-3.05041	2.21941
O	-1.84238	-2.44629	2.66323
H	-1.93242	-2.81082	3.55644
H	2.98901	-3.17327	0.66789
O	2.72489	-3.10694	1.61370
H	2.66371	-2.15082	1.76841
H	-5.28427	1.06205	-3.31813
O	-4.92301	0.71714	-2.48893
H	-5.49917	-0.02762	-2.25599

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Cysteine

N	-1.587438	1.627114	-0.332492
C	-0.524402	0.647391	-0.468101
C	-1.079083	-0.710225	-0.009264
O	-1.987819	-0.812250	0.779055
H	-0.230989	0.570069	-1.524934
C	0.749369	1.006115	0.345527
H	1.077911	2.006449	0.047093
S	2.223724	-0.072280	0.050885
H	0.525559	1.035261	1.415847
H	1.928146	-1.021334	0.963727
H	-2.128195	1.421643	0.505410
H	-1.219398	2.572715	-0.268429
O	-0.461967	-1.805332	-0.502483
H	0.302434	-1.537148	-1.046965

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Cystine

C	-2.809001	0.326811	0.092440
C	-3.646810	-0.959331	0.029838
O	-3.991874	-1.519408	-0.986531
O	-3.971013	-1.417481	1.265498
C	-1.445890	-0.004397	0.732959
S	-0.407261	1.479909	1.071499
N	-2.646920	0.966789	-1.199338
H	-3.338051	1.019194	0.759453
H	-4.491854	-2.231636	1.128011

H	-0.862623	-0.684055	0.102124
H	-1.601969	-0.478582	1.707035
H	-3.561835	1.182167	-1.591413
H	-2.212573	0.312703	-1.849194
C	2.224406	-0.462754	0.007945
C	3.663199	-0.978548	0.132794
O	4.115225	-1.924665	-0.473887
O	4.386655	-0.268326	1.030924
C	2.248514	1.015321	-0.420951
S	0.601916	1.794669	-0.721117
N	1.405249	-1.288491	-0.868122
H	1.794611	-0.497607	1.018841
H	5.273482	-0.675706	1.055019
H	2.758772	1.126430	-1.387715
H	2.804884	1.596165	0.316874
H	1.623777	-2.268470	-0.692225
H	1.672136	-1.125518	-1.838888