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Supporting information for:

Evaluation of the aggregation process in a mixture of propofol and benzocaine

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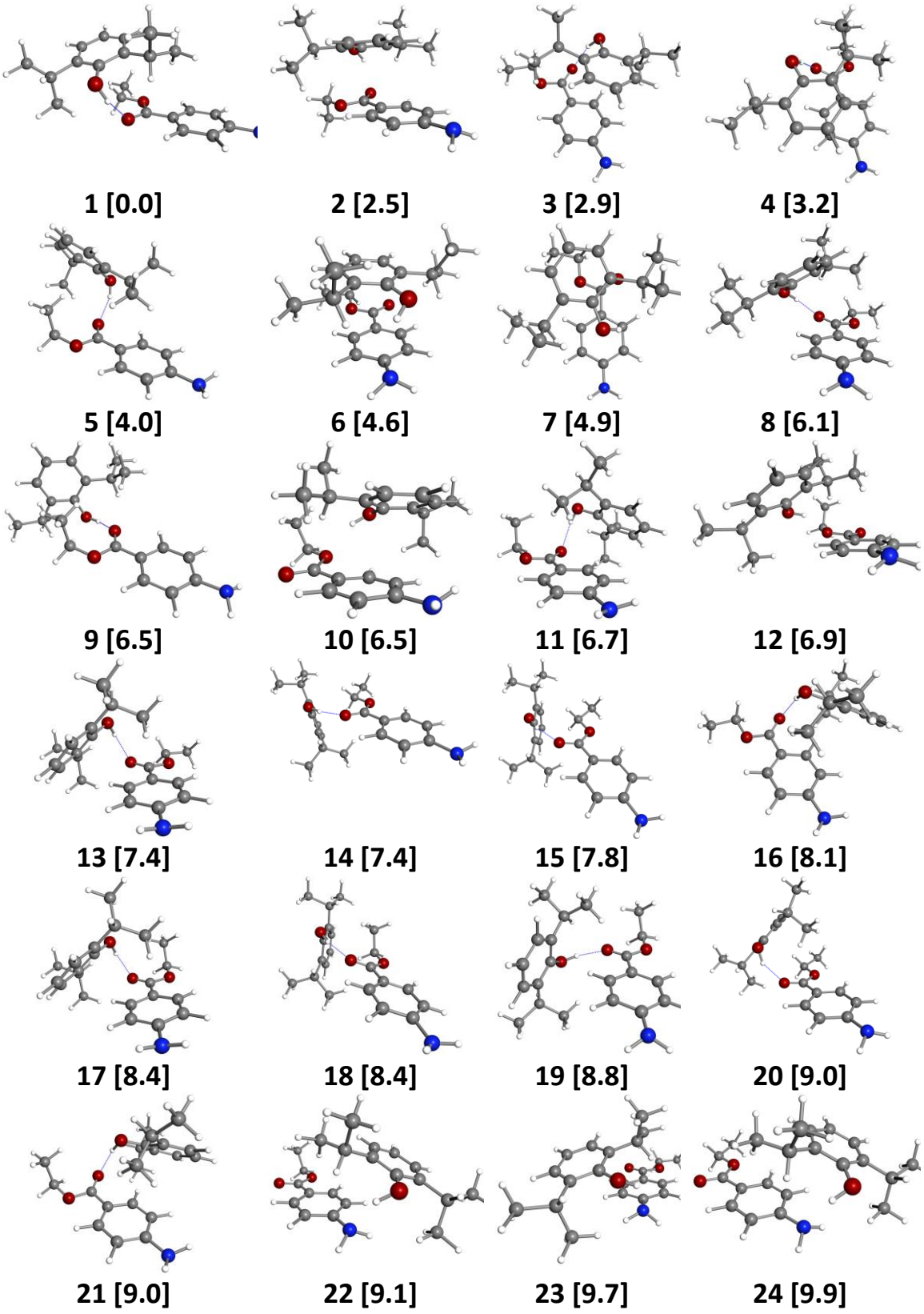
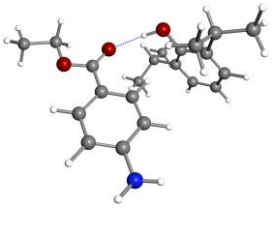
Reference S1

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Farkas, J. B. Foresman, J. V Ortiz, J. Cioslowski and D. J. Fox, *Gaussian 09, Revis. D.01, Gaussian, Inc., Wallingford CT*, 2009

Figure S1. Calculated structures of propofol•benzocaine at M06-2X/6-311+G(d) level, together with their relative stability in kJ/mol. ZPE correction was applied to all the energy values.





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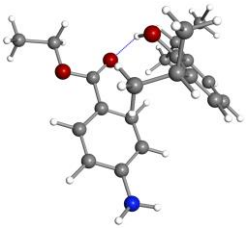

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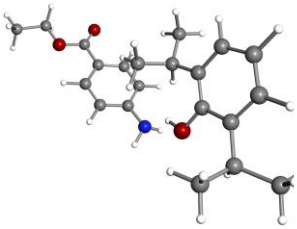

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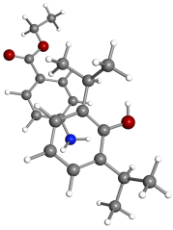

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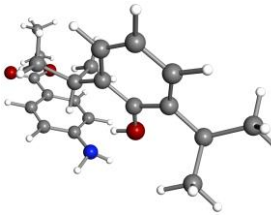

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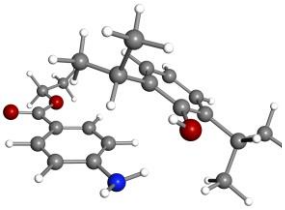

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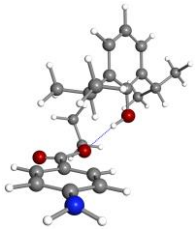

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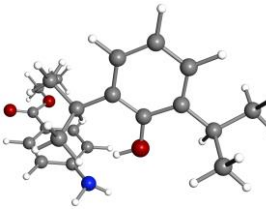

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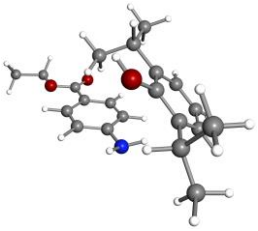

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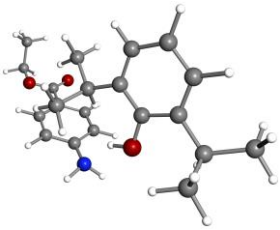

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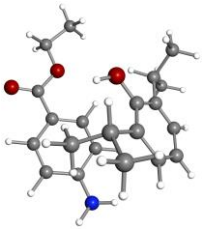

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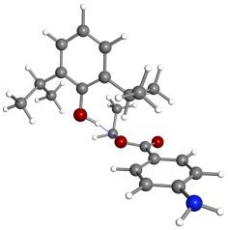

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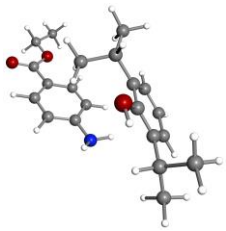

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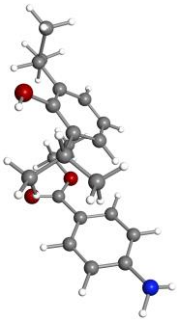

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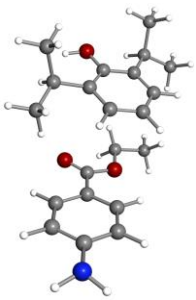

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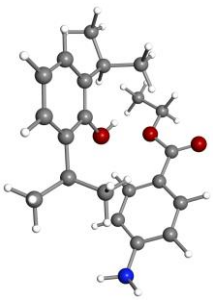

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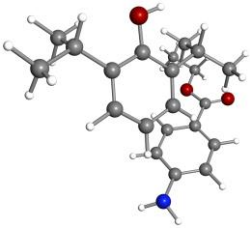

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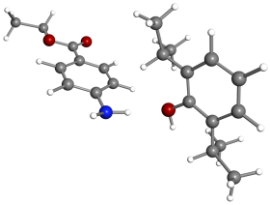

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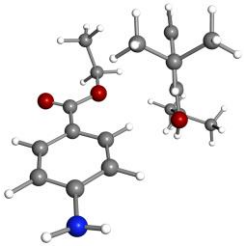

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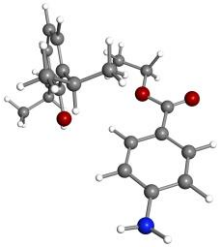


44 [29.1]

Table S1. Calculated structures propofol•benzocaine at M06-2X/6-31+G(d) level, together with their relative stability in kJ/mol.

Structure	*ΔE (kJ/mol)*	*ΔE_{ZPE} (kJ/mol)*	*$\Delta G_{298.15}$ (kJ/mol)*
1	0.0	0.0	3.0
2	2.3	2.5	7.4
3	3.9	2.9	6.7
4	3.5	3.2	5.3
5	3.6	4.0	5.4
6	2.2	4.6	11.4
7	6.5	4.9	14.0
8	7.2	6.1	3.5
9	6.4	6.5	5.6
10	5.3	6.5	12.3
11	6.6	6.7	8.5
12	7.9	6.9	7.4
13	7.8	7.4	6.0
14	8.2	7.4	2.5
15	8.3	7.8	0.3
16	7.6	8.1	12.8
17	8.9	8.4	6.9
18	7.0	8.4	9.5
19	9.3	8.8	3.9
20	9.7	9.0	3.0
21	7.2	9.0	11.0
22	8.8	9.1	7.4
23	9.0	9.7	9.7
24	8.5	9.9	9.3
25	9.9	10.0	13.2
26	9.4	10.4	12.1
27	9.8	11.6	14.5
28	12.3	12.0	8.2
29	10.2	12.3	11.2
30	15.2	14.0	11.6
31	12.8	14.2	17.0
32	13.3	14.8	17.0
33	15.7	14.8	11.4
34	13.1	14.9	10.1
35	16.2	15.6	14.2
36	15.3	16.1	16.9
37	20.0	19.4	15.7
38	22.0	21.4	21.8
39	21.1	21.4	18.4
40	23.2	21.9	22.1
41	25.7	24.7	22.3
42	25.1	25.2	18.5
43	26.4	26.0	26.9
44	29.2	29.1	27.4

Figure S2. Experimental IDIRS of propofol•benzocaine (upper trace) together with the predicted frequencies for each calculated structure at M06-2X/6-31+G(d) level. A correction factor of 0.955 was employed.

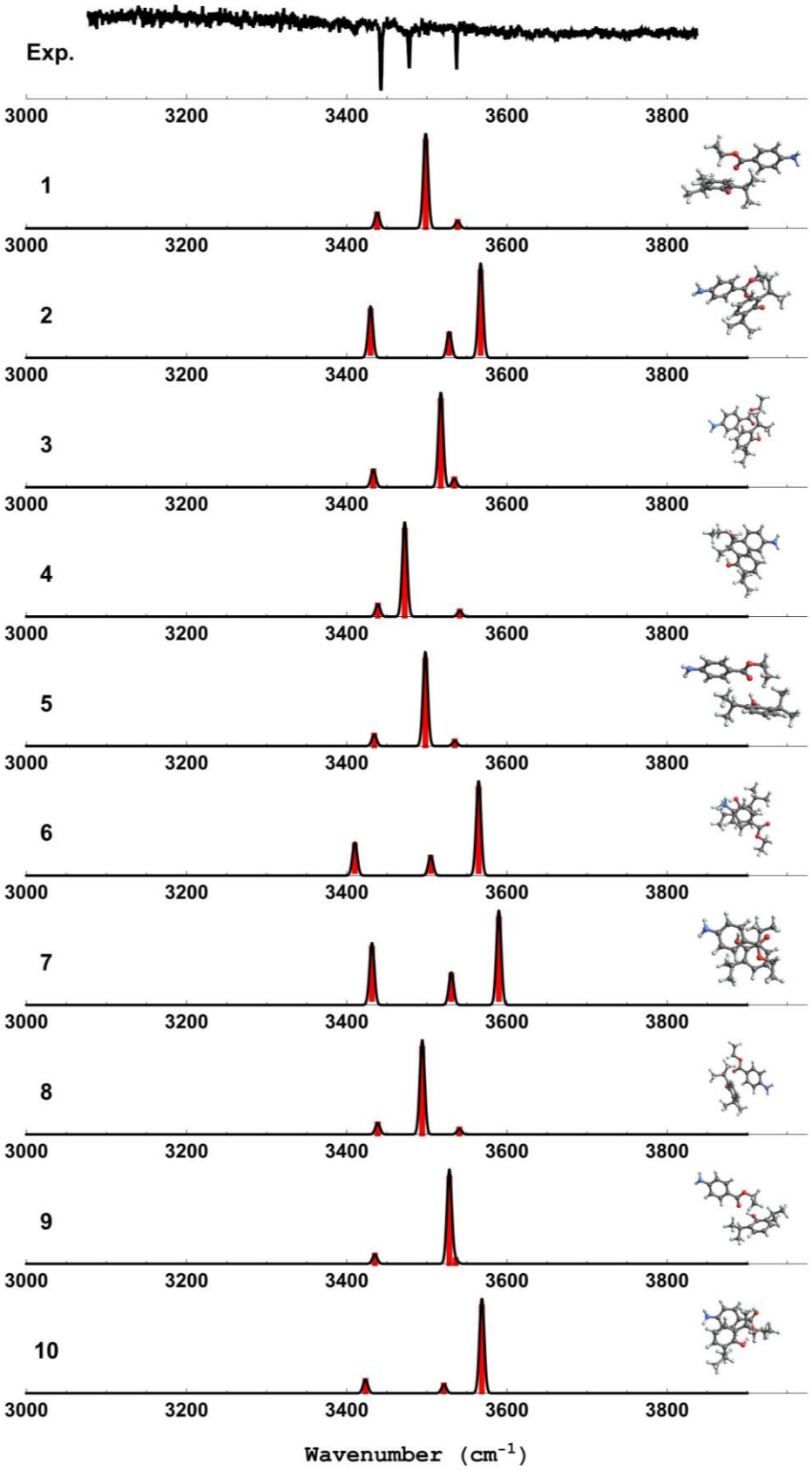


Figure S2. Cont.

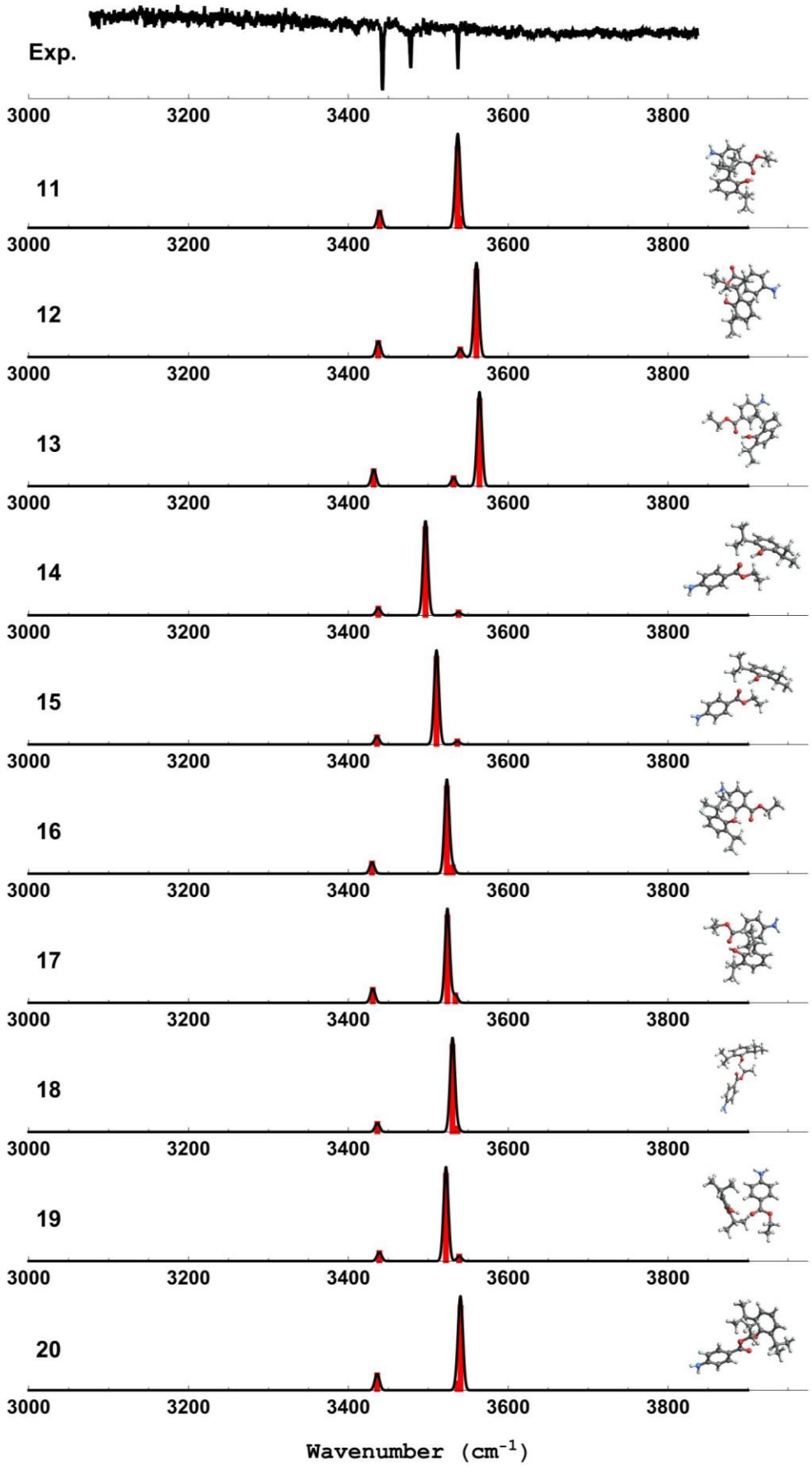


Figure S2. Cont.

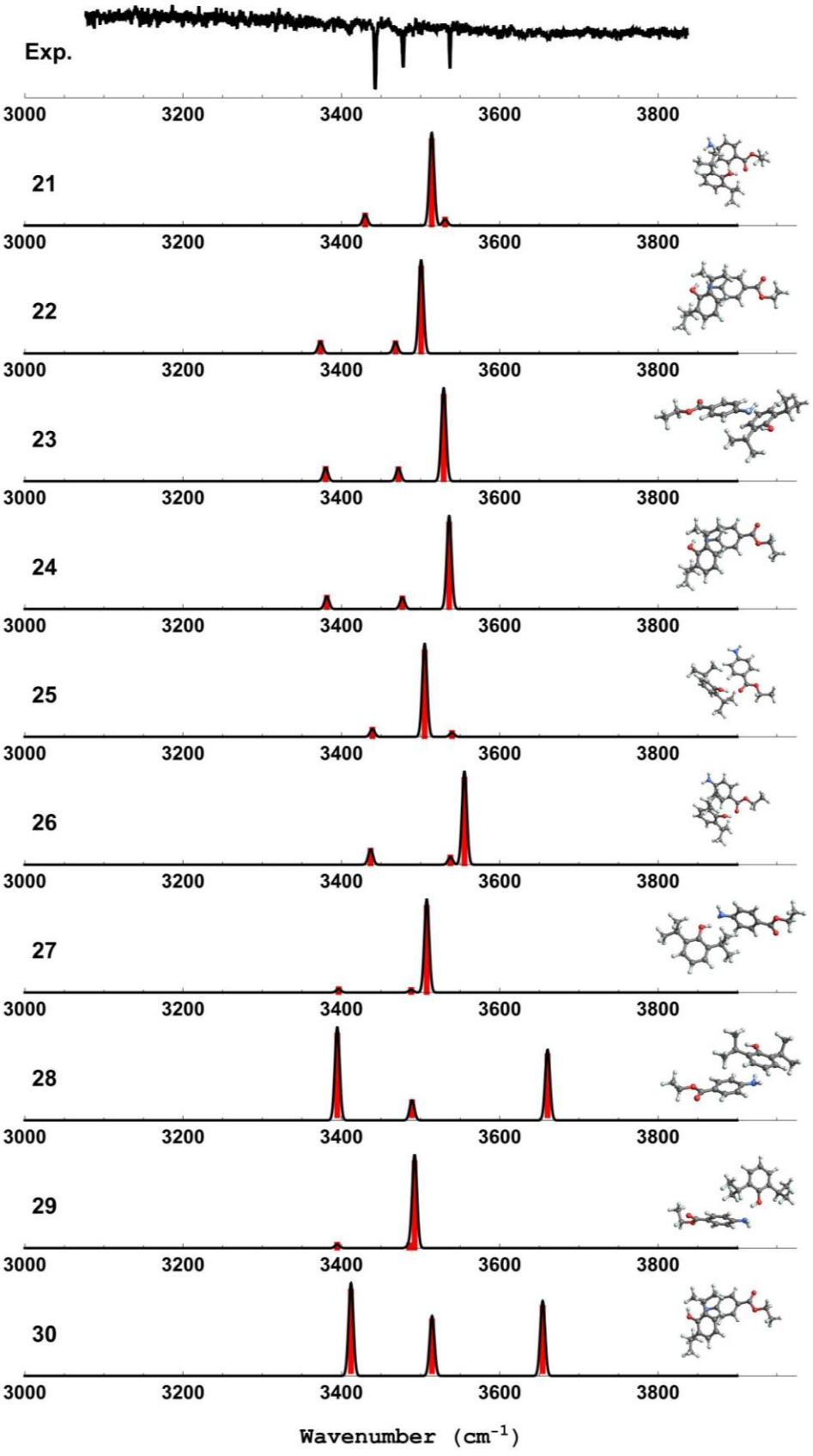


Figure S2. Cont.

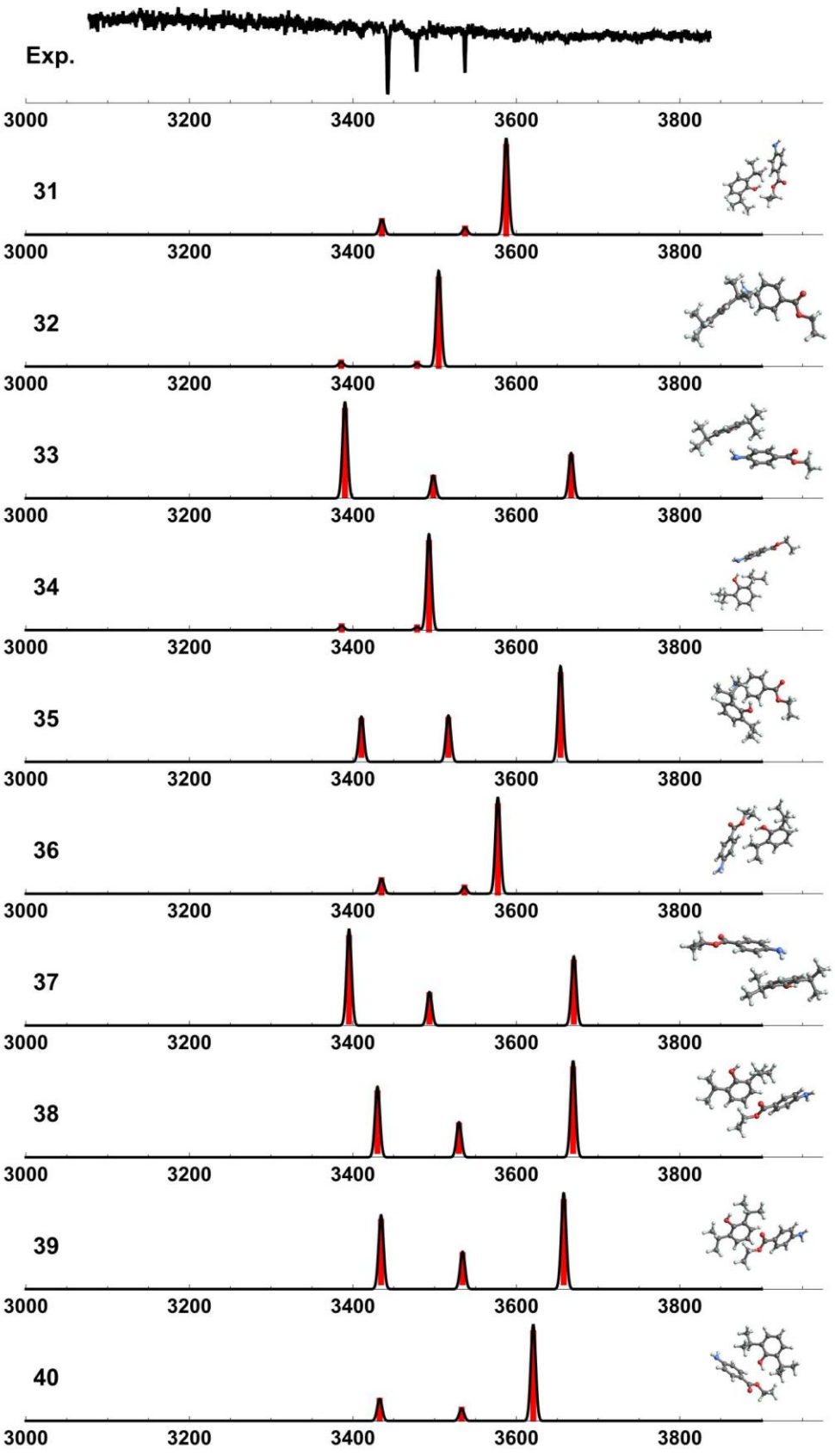

Exp.
3000
3200
3400
3600
3800
31
32
33
34
35
36
37
38
39
40
Wavenumber (cm-1)

Figure S2. Cont.

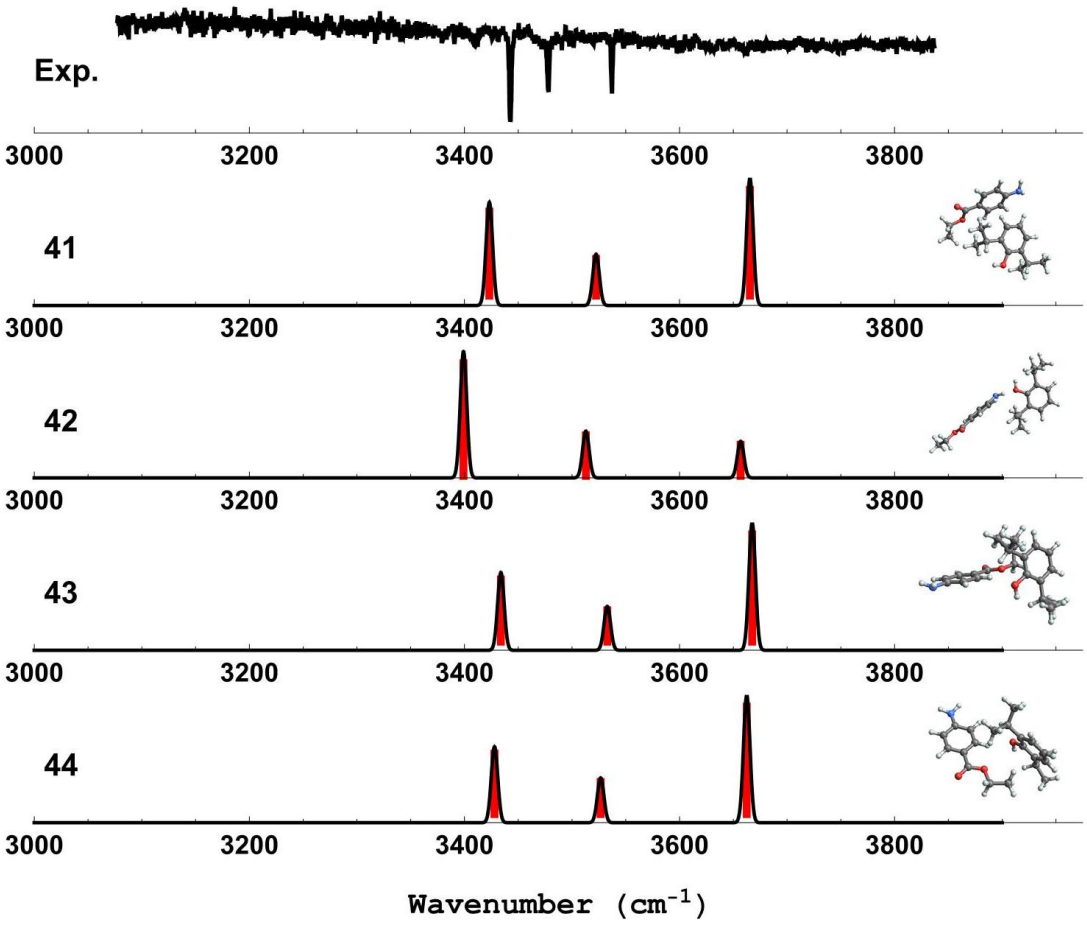
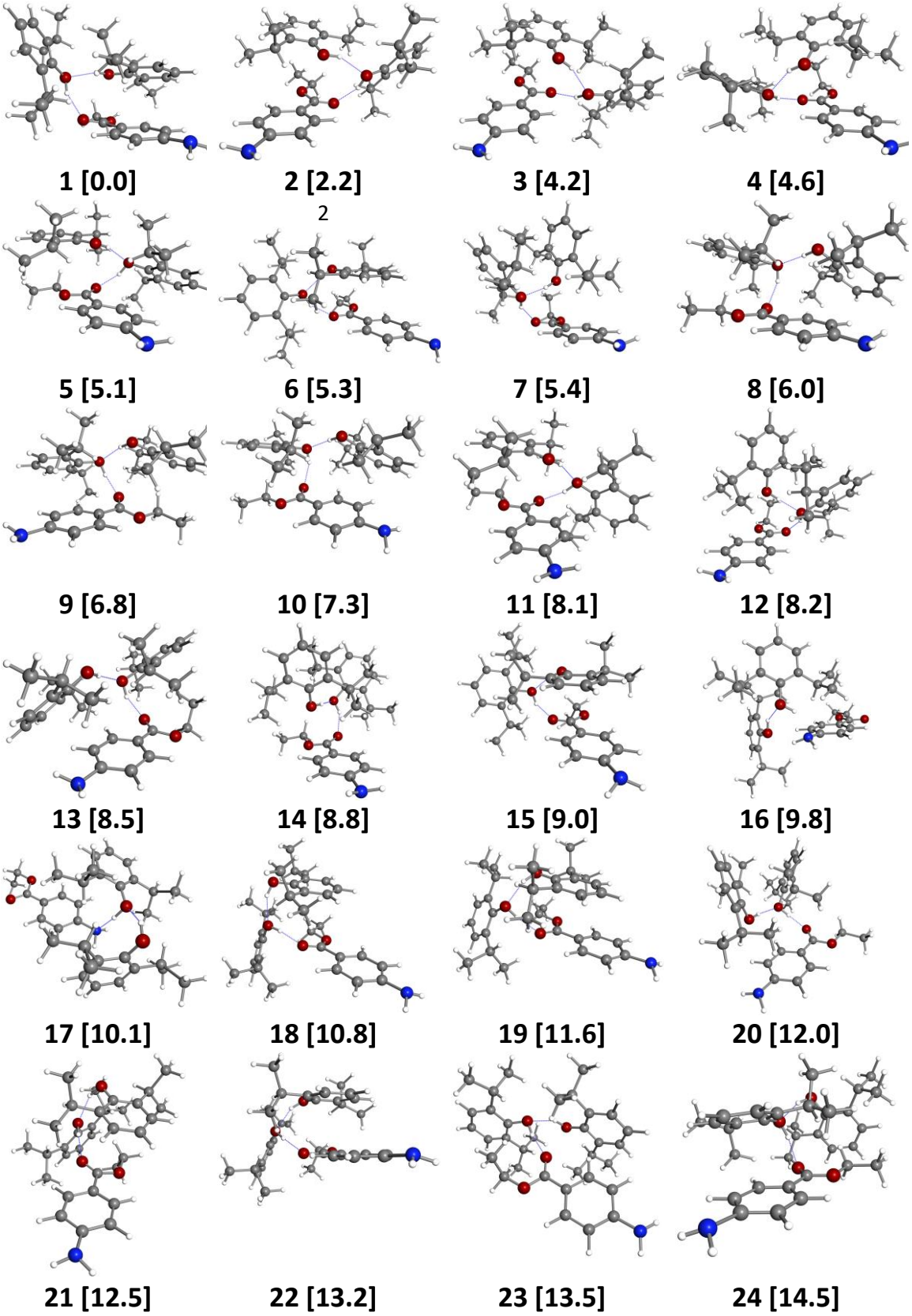
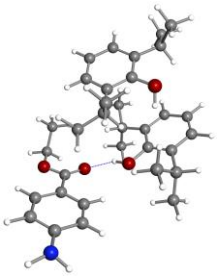


Figure S3. Calculated structures of propofol$_2$•benzocaine at M06-2X/6-311+G(d) level, together with their relative stability in kJ/mol. ZPE correction was applied to all the energy values.





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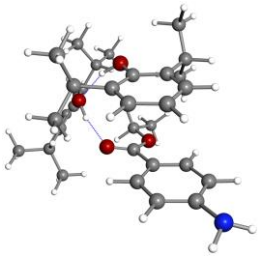

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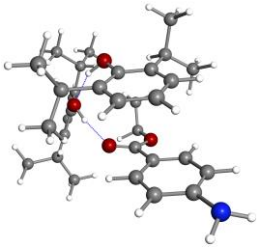

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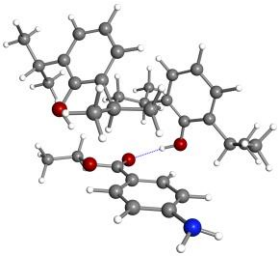

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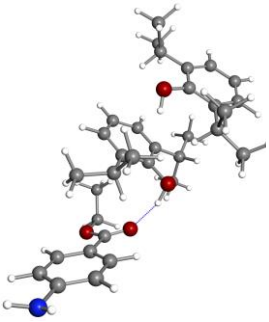

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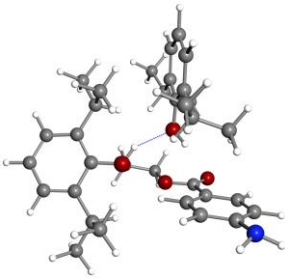

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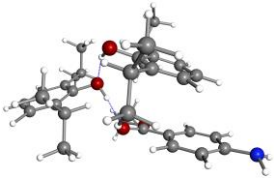

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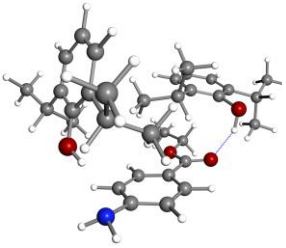

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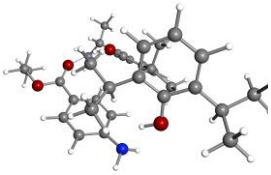

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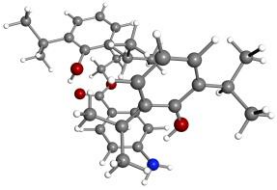

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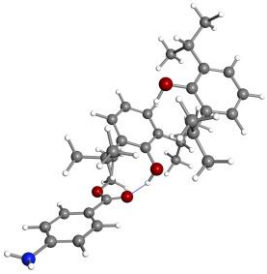

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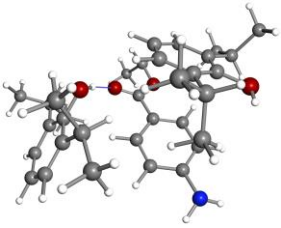

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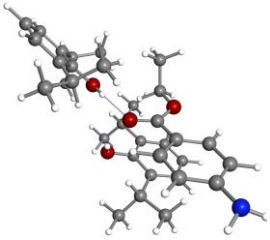

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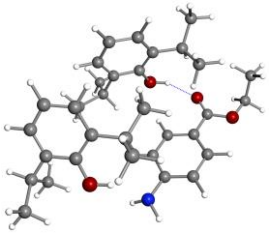

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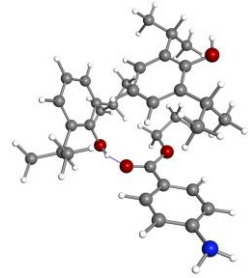

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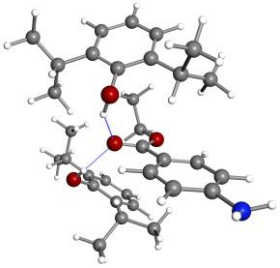

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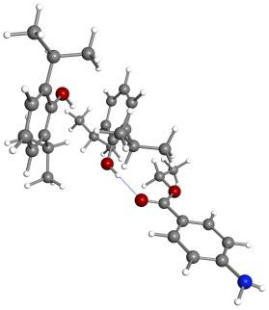

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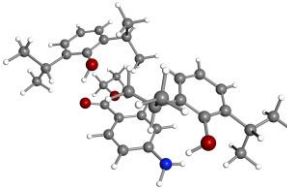

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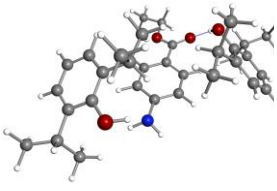

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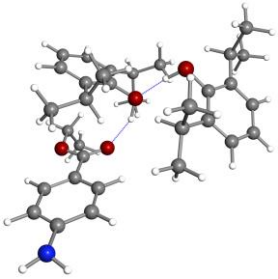
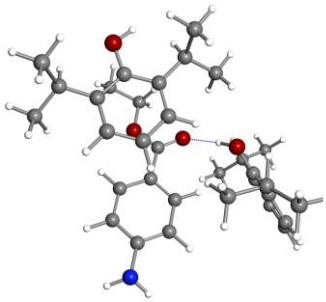
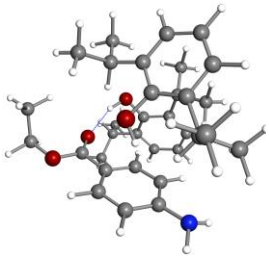


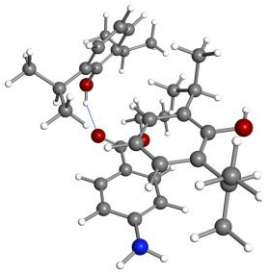
44 [32.7]



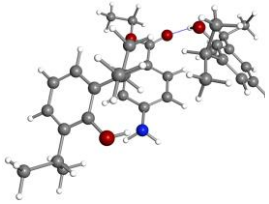
45 [33.2]



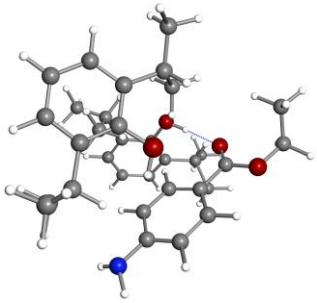
46 [33.4]



47 [33.5]



48 [34.5]



49 [37.1]

Table S2. Calculated structures propofol$_2$•benzocaine at M06-2X/6-31+G(d) level, together with their relative stability in kJ/mol.

Structure	*ΔE (kJ/mol)*	*ΔE_{ZPE} (kJ/mol)*	*$\Delta G_{298.15}$ (kJ/mol)*
1	0.0	0.0	0.0
2	4.0	2.2	0.9
3	2.9	4.2	4.6
4	2.5	4.6	8.3
5	6.8	5.1	7.1
6	6.2	5.3	3.0
7	8.1	5.4	7.5
8	6.9	6.0	9.3
9	9.3	6.8	8.0
10	7.8	7.3	11.7
11	10.0	8.1	4.6
12	9.2	8.2	12.8
13	9.1	8.5	12.9
14	10.6	8.8	8.8
15	9.1	9.0	8.9
16	9.2	9.8	2.7
17	11.4	10.1	15.2
18	12.7	10.8	8.1
19	12.5	11.6	10.5
20	11.8	12.0	14.1
21	12.9	12.5	14.7
22	13.3	13.2	12.9
23	16.1	13.5	10.4
24	14.1	14.5	21.5
25	20.6	15.4	11.1
26	19.8	16.1	10.0
27	20.4	19.0	17.7
28	22.5	20.1	23.3
29	24.9	22.2	20.1
30	23.7	23.1	26.7
31	28.1	24.3	15.4
32	25.7	24.9	21.9
33	26.5	25.8	23.7
34	27.6	26.8	25.4
35	28.6	26.8	26.1
36	31.3	28.3	27.6
37	28.8	28.3	27.3
38	29.5	28.8	31.6
39	32.6	29.9	27.6
40	32.8	30.5	28.1
41	34.3	30.8	23.0
42	33.4	32.0	28.9
43	33.1	32.7	27.3
44	36.4	32.7	28.9
45	35.5	33.2	29.6

46	38.0	33.4	32.3
47	35.5	33.5	33.1
48	35.5	34.5	26.9
49	40.8	37.1	31.6

Figure S4. Experimental IDIRS of propofol$_2$•benzocaine (upper trace) together with the predicted frequencies for each calculated structure at M06-2X/6-31+G(d) level. A correction factor of 0.955 was employed.

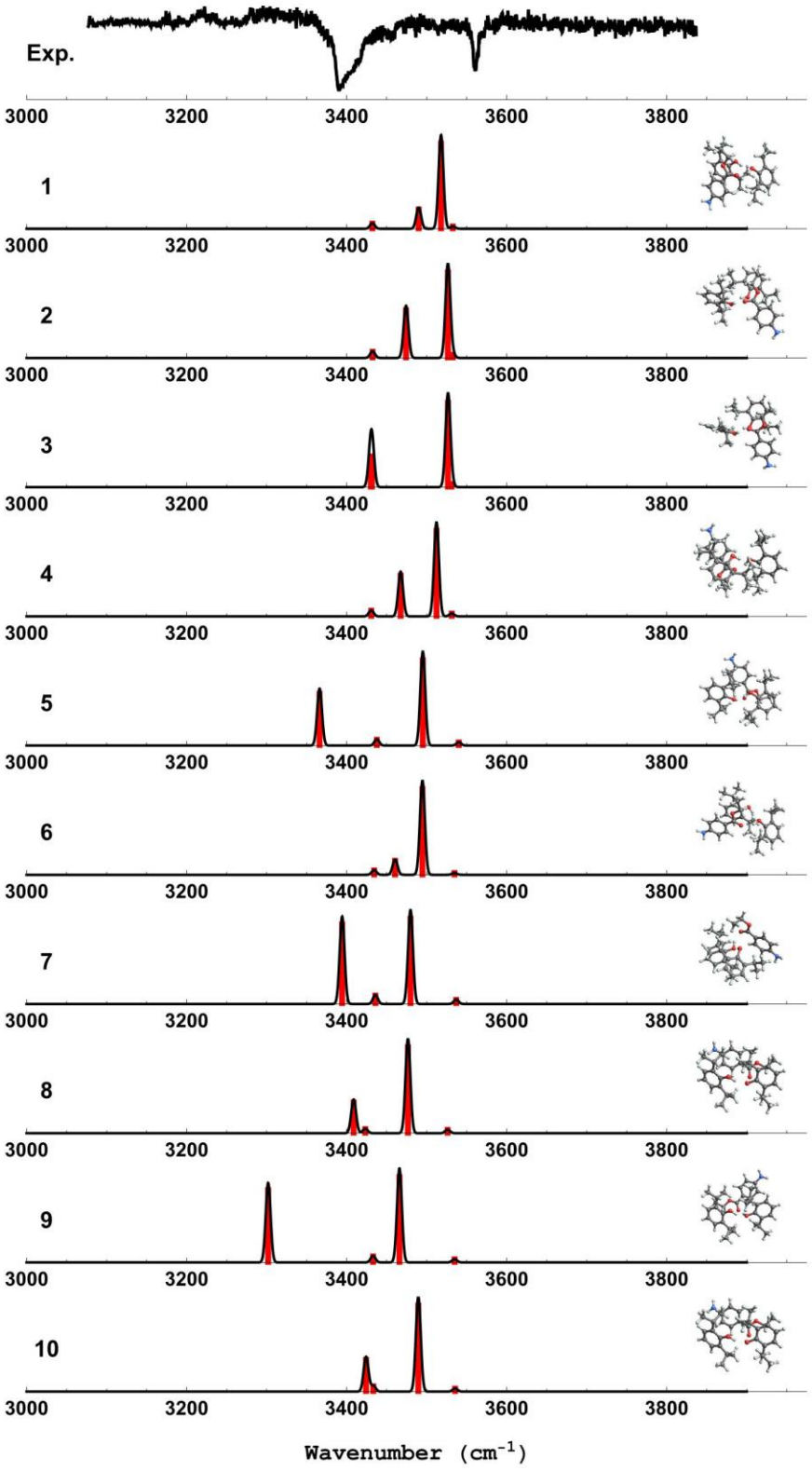


Figure S4. Cont.

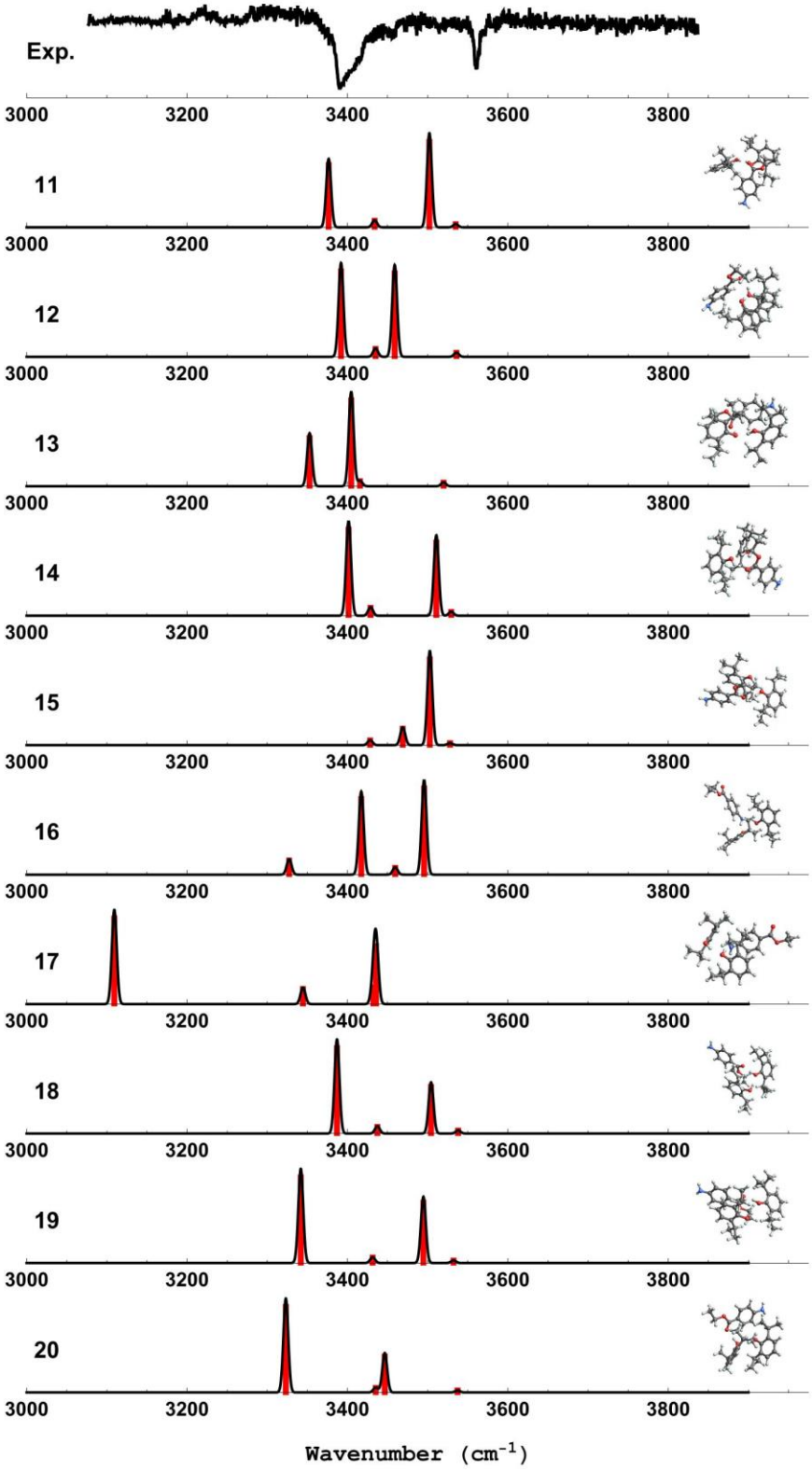


Figure S4. Cont.

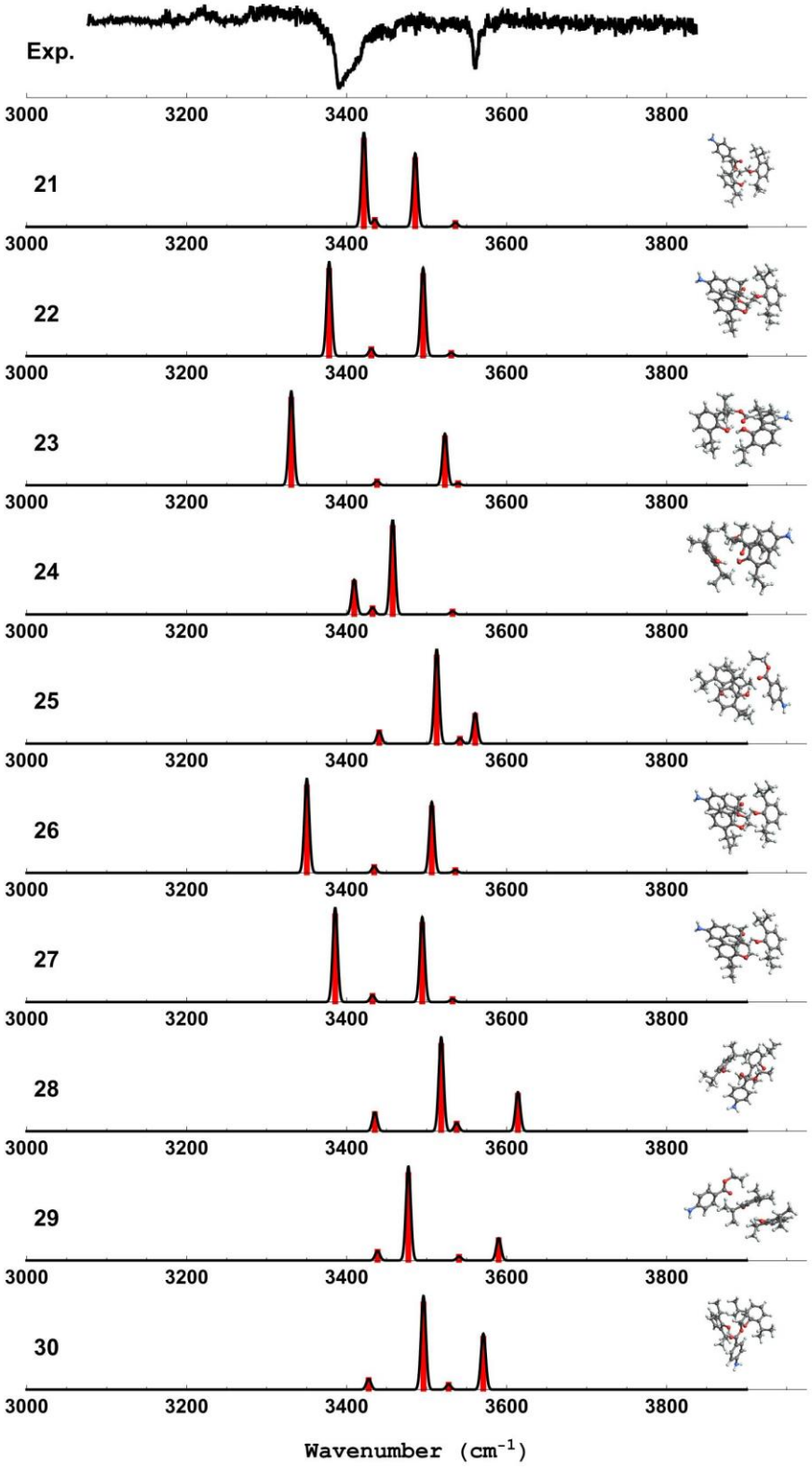


Figure S4. Cont.

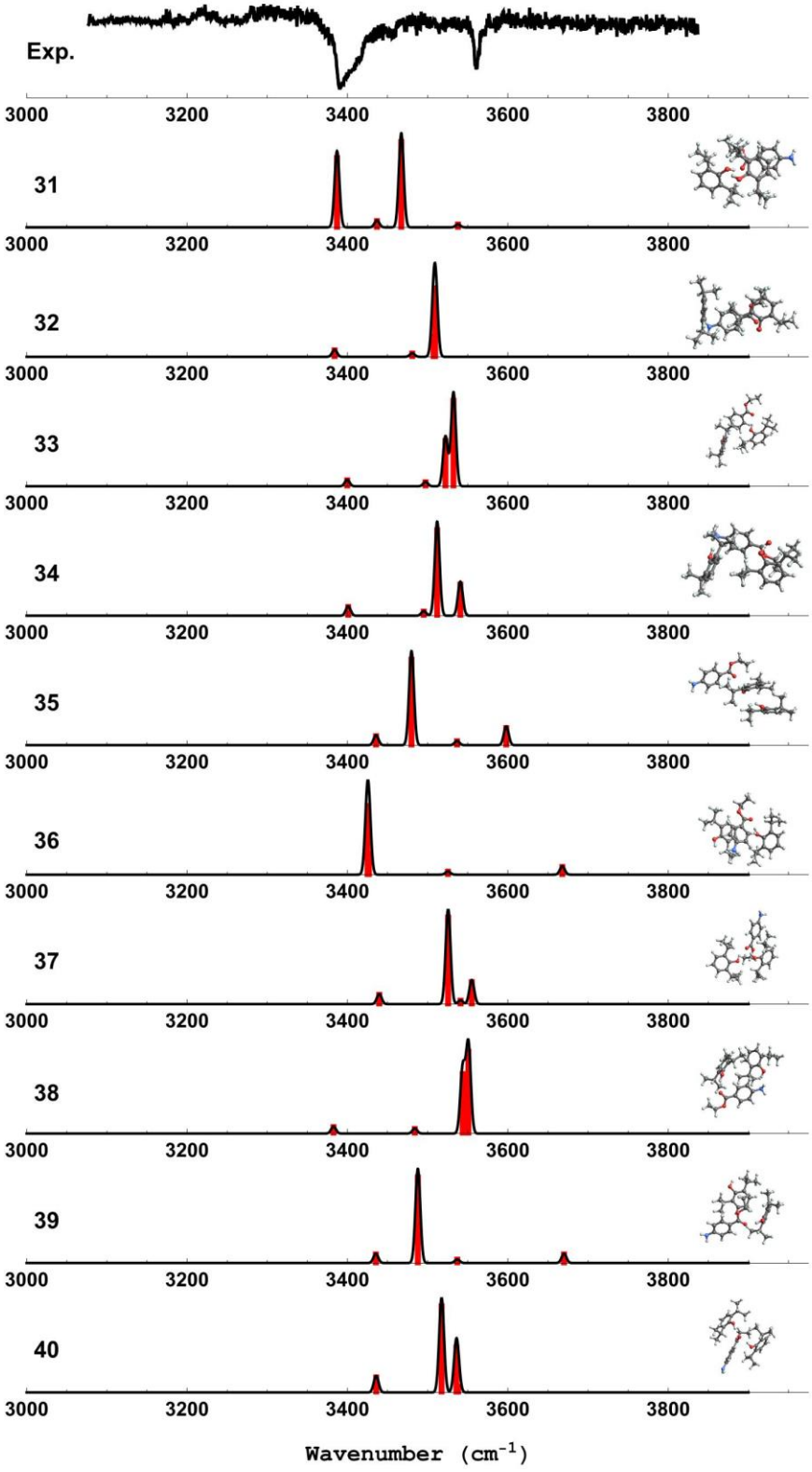


Figure S4. Cont.