Supporting Information

Rational Design of a Dummy-Imprinted Nanoplatform for Ultrasensitive and Leakage-Free Headspace-Electrochemical Detection of 2-MIB

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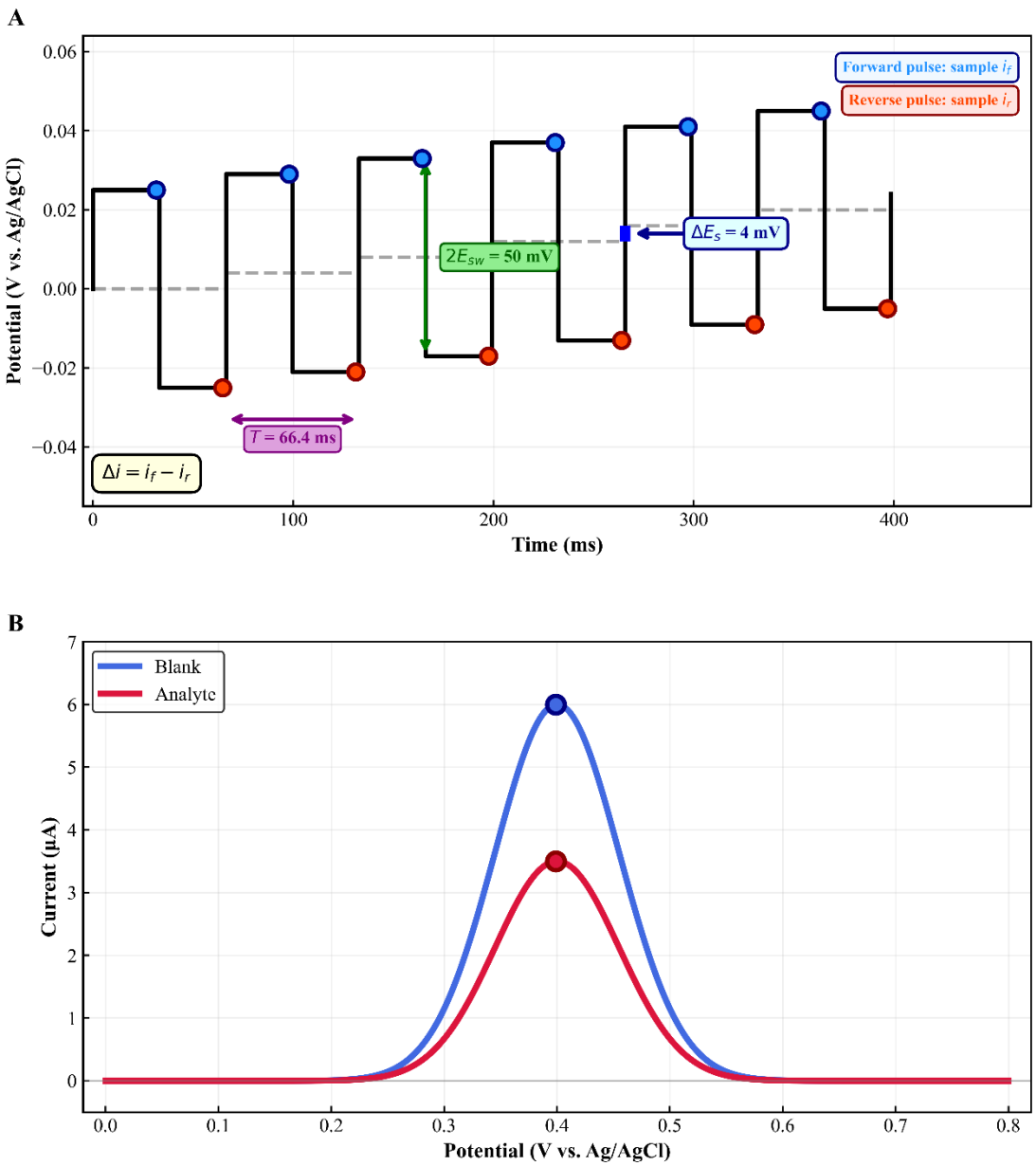

Fig. S1. Schematic Illustration of the Square Wave Voltammetry (SWV) Mechanism and Signal Quantification Strategy.

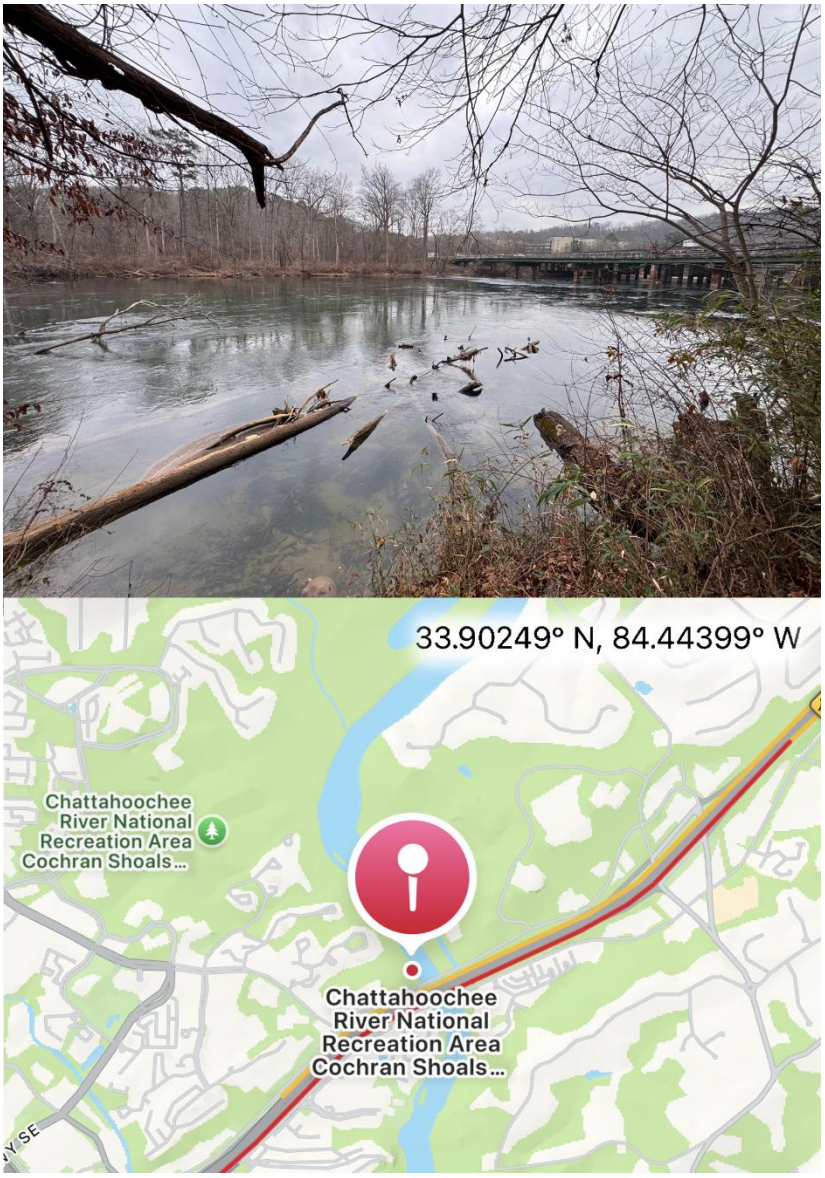

Fig. S2. On-Site Sampling Location and Environmental Context of the Chattahoochee River (Georgia, USA).

Table S1. Physicochemical characteristics of the different water matrices used for environmental validation

Sample Type	Source	pH	Conductivity (µS/cm)
Bottled Spring Water (BSW)	Local Supermarket	7.54	7.156
River Water (RW)	Chattahoochee River, GA	8.21	2524

Table S2. Full Screening Ranked by Topological Torsion Similarity to 2-MIB

CID	Name	SMILES	Candidate	Topological Torsion	Rank
16913	1,2,7,7-tetramethylbicyclo[2.2.1]heptan-2-ol	CC1(C2CCC1(C(C2)(C)O)C)C	FALSE	1	1
11062802	(1R,2R,4R)-1,2,7,7-tetramethylbicyclo[2.2.1]heptan-2-ol	CC1(C2CCC1(C(C2)(C)O)C)C	FALSE	1	2
12648890	1,2,3,3-tetramethylbicyclo[2.2.1]heptan-2-ol	CC1(C2CCC(C2)(C1(C)O)C)C	FALSE	0.6667	3
106997	2-Ethylfenchol	CCC1(C(C2CCC1(C2)C)(C)C)O	TRUE	0.587	4
76959240	(1R,2R,4S)-2-ethyl-1,3,3-trimethylbicyclo[2.2.1]heptan-2-ol	CCC1(C(C2CCC1(C2)C)(C)C)O	FALSE	0.587	5
1753956	(3R,6S,9S)-2,2,8,8-tetramethyl-octahydro-1H-2,4a-methanonapthalen-9-ol	CC1(CCCC2(C13CCC(C3)C2(C)C)O)C	FALSE	0.5	6
534931	2,2,8,8-tetramethyl-octahydro-1H-2,4a-methanonapthalen-9-ol	CC1(CCCC2(C13CCC(C3)C2(C)C)O)C	FALSE	0.5	7
11043252	(1'R,2S,4S,4'R)-1',7',7'-trimethyl-2-propan-2-ylspiro[1,3-dioxane-4,2'-bicyclo[2.2.1]heptane]	CC(C)C1OCCC2(O1)CC3CCC2(C3(C)C)C	FALSE	0.4828	8
107035	2,2,8,8-tetramethyl-6-oxatetracyclo[7.2.1.01,7.05,7]dodecane	CC1(CCC2C3(C14CCC(C4)C3(C)C)O2)C	FALSE	0.403	9
10955174	(1R,3R,6S,7S,8S)-2,2,6,8-tetramethyltricyclo[5.3.1.03,8]undecan-3-ol	CC1CCC2(C(C3CCC2(C1C3)C)(C)C)O	FALSE	0.3934	10

521903	2,2,6,8-tetramethyltricyclo[5.3.1.03,8]undecan-3-ol	CC1CCC2(C(C3CCC2(C1C3)C)(C)C)O	FALSE	0.3934	11
442384	(6S,8S)-2,2,6,8-tetramethyltricyclo[5.3.1.03,8]undecan-3-ol	CC1CCC2(C(C3CCC2(C1C3)C)(C)C)O	FALSE	0.3934	12
12242824	(1R,4S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-ol	CC1(C2CCC1(C(C2)O)C)C	FALSE	0.3469	13
44630107	(2S,4R)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-ol	CC1(C2CCC1(C(C2)O)C)C	FALSE	0.3469	14
18639728	(1S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-ol	CC1(C2CCC1(C(C2)O)C)C	FALSE	0.3469	15
6973640	(1S,2S,4S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-ol	CC1(C2CCC1(C(C2)O)C)C	FALSE	0.3469	16
439568	(2S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-ol	CC1(C2CCC1(C(C2)O)C)C	FALSE	0.3469	17
512289	(1R,2R)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-ol	CC1(C2CCC1(C(C2)O)C)C	FALSE	0.3469	18
230920	(1S,2S,4R)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-ol	CC1(C2CCC1(C(C2)O)C)C	FALSE	0.3469	19
657014	(1R,4R)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-ol	CC1(C2CCC1(C(C2)O)C)C	FALSE	0.3469	20
6321405	(1R,2R,4R)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-ol	CC1(C2CCC1(C(C2)O)C)C	TRUE	0.3469	21
64685	1,7,7-trimethylbicyclo[2.2.1]heptan-2-ol	CC1(C2CCC1(C(C2)O)C)C	TRUE	0.3469	22

1201518	(1S,2R,4S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-ol	CC1(C2CCC1(C(C2)O)C)C	FALSE	0.3469	23
6552009	(1R,2S,4R)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-ol	CC1(C2CCC1(C(C2)O)C)C	FALSE	0.3469	24
18345891	(1R)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-ol	CC1(C2CCC1(C(C2)O)C)C	FALSE	0.3469	25
10049	(1S,2R,4R)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-ol	CC1(C2CCC1(C(C2)O)C)C	FALSE	0.3469	26
6850744	(1S,4S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-ol	CC1(C2CCC1(C(C2)O)C)C	FALSE	0.3469	27
439569	(2R)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-ol	CC1(C2CCC1(C(C2)O)C)C	FALSE	0.3469	28
95330	2-methoxy-1,7,7-trimethylbicyclo[2.2.1]heptane	CC1(C2CCC1(C(C2)OC)C)C	FALSE	0.3333	29
518472	(1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl) formate	CC1(C2CCC1(C(C2)OC=O)C)C	FALSE	0.3269	30
23623868	[(1R,2R,4R)-1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl] formate	CC1(C2CCC1(C(C2)OC=O)C)C	FALSE	0.3269	31
22211593	[(1S,2R,4S)-1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl] formate	CC1(C2CCC1(C(C2)OC=O)C)C	FALSE	0.3269	32
13428328	[(1R,2S,4R)-1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl] formate	CC1(C2CCC1(C(C2)OC=O)C)C	FALSE	0.3269	33
6448	(1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl) acetate	CC(=O)OC1CC2CCC1(C2(C)C)C	FALSE	0.3208	34
6950273	[(1S,2S,4S)-1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl] acetate	CC(=O)OC1CC2CCC1(C2(C)C)C	FALSE	0.3208	35

93009	[(1S,2R,4S)-1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl] acetate	CC(=O)OC1CC2CCC1(C2(C)C)C	FALSE	0.3208	36
442460	[(2R)-1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl] acetate	CC(=O)OC1CC2CCC1(C2(C)C)C	FALSE	0.3208	37
13750367	2-[(1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl)oxy]ethanol	CC1(C2CCC1(C(C2)OCCO)C)C	FALSE	0.3208	38
443131	[(2S)-1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl] acetate	CC(=O)OC1CC2CCC1(C2(C)C)C	FALSE	0.3208	39
637531	[(1R,2R,4R)-1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl] acetate	CC(=O)OC1CC2CCC1(C2(C)C)C	FALSE	0.3208	40
1.32E+08	[(1S,2R)-1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl] acetate	CC(=O)OC1CC2CCC1(C2(C)C)C	FALSE	0.3208	41
6950274	[(1R,2S,4R)-1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl] acetate	CC(=O)OC1CC2CCC1(C2(C)C)C	FALSE	0.3208	42
111255	2-[[(1S,2S,4S)-1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl]oxy]ethanol	CC1(C2CCC1(C(C2)OCCO)C)C	FALSE	0.3208	43
23617863	[(1S,2S,4S)-1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl] propanoate	CCC(=O)OC1CC2CCC1(C2(C)C)C	FALSE	0.3091	44
23617864	[(1R,2R,4R)-1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl] propanoate	CCC(=O)OC1CC2CCC1(C2(C)C)C	FALSE	0.3091	45
89306	(1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl) propanoate	CCC(=O)OC1CC2CCC1(C2(C)C)C	FALSE	0.3091	46
76966069	[(1S,2R,4S)-1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl] butanoate	CCCC(=O)OC1CC2CCC1(C2(C)C)C	FALSE	0.3036	47
97897	(1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl) butanoate	CCCC(=O)OC1CC2CCC1(C2(C)C)C	FALSE	0.3036	48

5315645	1,7-dimethyl-7-(4-methylpent-3-enyl)bicyclo[2.2.1]heptan-2-ol	CC(=CCCC1(C2CCC1(C(C2)O)C)C)C	FALSE	0.3036	49
18955245	2-methyl-3-[(1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl)oxy]propan-1-ol	CC(CO)COC1CC2CCC1(C2(C)C)C	FALSE	0.3036	50
174490	[(1R,2R,4R)-1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl] 2-methylpropanoate	CC(C)C(=O)OC1CC2CCC1(C2(C)C)C	FALSE	0.2982	51
60968	(1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl) 3-methylbutanoate	CC(C)CC(=O)OC1CC2CCC1(C2(C)C)C	FALSE	0.2982	52
91226	(1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl) 2-methylpropanoate	CC(C)C(=O)OC1CC2CCC1(C2(C)C)C	FALSE	0.2982	53
36690486	[(1S,2S,4S)-1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl] 3-methylbutanoate	CC(C)CC(=O)OC1CC2CCC1(C2(C)C)C	FALSE	0.2982	54
76957121	[(1R,2R,4R)-1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl] 3-methylbutanoate	CC(C)CC(=O)OC1CC2CCC1(C2(C)C)C	FALSE	0.2982	55
23623651	[(1S,2R,4S)-1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl] 3-methylbutanoate	CC(C)CC(=O)OC1CC2CCC1(C2(C)C)C	FALSE	0.2982	56
22082179	(1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl) 2-methylbutanoate	CCC(C)C(=O)OC1CC2CCC1(C2(C)C)C	FALSE	0.2881	57

610072	1,5,5,8-tetramethyltricyclo[5.4.0.04,8]undecan-7-ol	CC1(CC2(C3(CCCC2(C1CC3)C)C)O)C	FALSE	0.2879	58
3082861	(1R,4S,7R,8S)-1,5,5,8-tetramethyltricyclo[5.4.0.04,8]undecan-7-ol	CC1(CC2(C3(CCCC2(C1CC3)C)C)O)C	FALSE	0.2879	59
133454	(2aS,4aR,8R)-2,2,4a,8-tetramethyl-2a,3,4,5,6,7-hexahydro-1H-cyclobuta[i]inden-8-ol	CC1(CC23C1CCC2(CCCC3(C)O)C)C	FALSE	0.2879	60
106674	4-(1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl)cyclohexan-1-ol	CC1(C2CCC1(C(C2)C3CCC(CC3)O)C)C	FALSE	0.2698	61
16070753	1-(1,7,7-trimethyl-2-bicyclo[2.2.1]heptanyl)cyclohexan-1-ol	CC1(C2CCC1(C(C2)C3(CCCCC3)O)C)C	FALSE	0.2615	62
163417	1,5,8-trimethylbicyclo[3.2.1]octan-8-ol	CC12CCCC(C1(C)O)(CC2)C	FALSE	0.2593	63
242493	(3R,5S,8R,9S,10S,13S,14S,17S)-10,13,17-trimethyl-1,2,3,4,5,6,7,8,9,11,12,14,15,16-tetradecahydrocyclopenta[a]phenanthrene-3,17-diol	CC12CCC(CC1CCC3C2CCC4(C3CCC4(C)O)C)O	FALSE	0.2436	64
101819	(3S,5S,8R,9S,10S,13S,14S,17S)-10,13,17-trimethyl-1,2,3,4,5,6,7,8,9,11,12,14,15,16-tetradecahydrocyclopenta[a]phenanthrene-3,17-diol	CC12CCC(CC1CCC3C2CCC4(C3CCC4(C)O)C)O	FALSE	0.2436	65
15706076	(3R,5R,7R,8R,9S,10S,13S,14S,17S)-7,10,13,17-tetramethyl-	CC1CC2CC(CCC2(C3C1C4CCC(C4(CC3)C)(C)O)C)O	FALSE	0.2346	66

	1,2,3,4,5,6,7,8,9,11,12,14,15,16-tetradecahydrocyclopenta[a]phenanthrene-3,17-diol				
22096564	[1-methyl-2-[(1,2,2-trimethyl-3-bicyclo[3.1.0]hexanyl)methyl]cyclopropyl]methanol	CC1(C(CC2C1(C2)C)CC3CC3(C)CO)C	FALSE	0.2344	67
535224	1,7,7-trimethylbicyclo[2.2.1]heptane-2,5-diol	CC1(C2CC(C1(CC2O)C)O)C	FALSE	0.2321	68
11768995	(1R,2S,3R,4S)-1,7,7-trimethylbicyclo[2.2.1]heptane-2,3-diol	CC1(C2CCC1(C(C2O)O)C)C	FALSE	0.2281	69
101680	2,3,3-trimethylbicyclo[2.2.1]heptan-2-ol	CC1(C2CCC(C2)C1(C)O)C	FALSE	0.2264	70
6997371	(1R,2R,4S)-1,3,3-trimethylbicyclo[2.2.1]heptan-2-ol	CC1(C2CCC(C2)(C1O)C)C	FALSE	0.2075	71
15406	1,3,3-trimethylbicyclo[2.2.1]heptan-2-ol	CC1(C2CCC(C2)(C1O)C)C	FALSE	0.2075	72
6973643	(1R,2S,4S)-1,3,3-trimethylbicyclo[2.2.1]heptan-2-ol	CC1(C2CCC(C2)(C1O)C)C	FALSE	0.2075	73
439711	(1S,2S,4R)-1,3,3-trimethylbicyclo[2.2.1]heptan-2-ol	CC1(C2CCC(C2)(C1O)C)C	FALSE	0.2075	74
15559490	(4R,4aR,8aS)-4,8a-dimethyl-1,2,3,4,5,6,7,8-octahydronaphthalen-4a-ol	CC1CCCC2(C1(CCCC2)O)C	FALSE	0.2	75
10966107	(1R,3aS,4S,7aS)-5-ethenyl-1,3a,4,7a-tetramethyl-1,2,3,4,6,7-hexahydroinden-5-ol	CC1CCC2(C1(CCC(C2C)(C=C)O)C)C	FALSE	0.2	76
142315	3,7,7-trimethylbicyclo[4.1.0]heptan-3-ol	CC1(C2C1CC(CC2)(C)O)C	FALSE	0.2	77

1213	4,8a-dimethyl-1,2,3,4,5,6,7,8-octahydronaphthalen-4a-ol	CC1CCCC2(C1(CCCC2)O)C	FALSE	0.2	78
29746	(4S,4aS,8aR)-4,8a-dimethyl-1,2,3,4,5,6,7,8-octahydronaphthalen-4a-ol	CC1CCCC2(C1(CCCC2)O)C	FALSE	0.2	79
101967	(3R,5R,8R,9S,10S,13S,14S,17R)-17-[(1S)-1-hydroxyethyl]-10,13-dimethyl-1,2,3,4,5,6,7,8,9,11,12,14,15,16-tetradecahydrocyclopenta[a]phenanthrene-3,17-diol	CC(C1(CCC2C1(CCC3C2CCC4C3(CCC(C4)O)C)C)O)O	FALSE	0.1977	80
3032833	(3R,5R,8R,9S,10S,13S,14S,17R)-17-(1-hydroxyethyl)-10,13-dimethyl-1,2,3,4,5,6,7,8,9,11,12,14,15,16-tetradecahydrocyclopenta[a]phenanthrene-3,17-diol	CC(C1(CCC2C1(CCC3C2CCC4C3(CCC(C4)O)C)C)O)O	FALSE	0.1977	81
107217	(1,3,3-trimethyl-2-bicyclo[2.2.1]heptanyl) acetate	CC(=O)OC1C(C2CCC1(C2)C)(C)C	FALSE	0.193	82
6427102	[(2S)-1,3,3-trimethyl-2-bicyclo[2.2.1]heptanyl] acetate	CC(=O)OC1C(C2CCC1(C2)C)(C)C	FALSE	0.193	83
14019266	[(1S,2S,4R)-1,3,3-trimethyl-2-bicyclo[2.2.1]heptanyl] acetate	CC(=O)OC1C(C2CCC1(C2)C)(C)C	FALSE	0.193	84
21145050	(1S,4S,5S)-5-hydroxy-1,7,7-trimethylbicyclo[2.2.1]heptan-2-one	CC1(C2CC(=O)C1(CC2O)C)C	TRUE	0.1897	85
189214	5-hydroxy-4,7,7-trimethylbicyclo[2.2.1]heptan-2-one	CC1(C2CC(C1(CC2=O)C)O)C	FALSE	0.1897	86

447414	(1R,4R,5R)-5-hydroxy-1,7,7-trimethylbicyclo[2.2.1]heptan-2-one	CC1(C2CC(=O)C1(CC2O)C)C	TRUE	0.1897	87
89145281	5,7,8-trimethyltricyclo[5.2.1.02,6]decan-8-ol	CC1CCC2C1C3(CC2CC3(C)O)C	FALSE	0.1846	88
163418	8-ethyl-1,5-dimethylbicyclo[3.2.1]octan-8-ol	CCC1(C2(CCCC1(CC2)C)C)O	FALSE	0.1833	89
521200	2,6,6,9-tetramethyltricyclo[5.4.0.02,9]undecan-8-ol	CC1(CCCC2(C3C1C(C2(CC3)C)O)C)C	FALSE	0.1831	90
637210	(1R,2R,5R,6R,9S,12S,13R)-6,9,12-trimethyl-5-propan-2-yltetracyclo[7.5.0.01,13.02,6]tetradecan-12-ol	CC(C)C1CCC2C1(CCC3(C24CC4C(CC3)(C)O)C)C	FALSE	0.1765	91
90658579	2-[(3S,3aS,5aR,5bR,7aS,11aS,11bR,13aR,13bS)-5a,5b,8,8,10,11a,13b-heptamethyl-1,2,3,3a,4,5,6,7,7a,9,10,11,11b,12,13,13a-hexadecahydrocyclopenta[a]chrysen-3-yl]propan-2-ol	CC1CC(C2CCC3(C(C2(C1)C)CCC4C3(CCC5C4(CCC5C(C)(C)O)C)C)C)(C)C	FALSE	0.1727	92
10775424	(1S,4S,7S,8R,11R)-2,2,4,8-tetramethyltricyclo[5.3.1.04,11]undecan-11-ol	CC1CCC2C(CC3(C2(C1CC3)O)C)(C)C	FALSE	0.169	93
164874	2-[(3S,3aS,5aR,5bR,7aS,11aS,11bR,13aR,13bS)-5a,5b,8,8,11a,13b-hexamethyl-	CC1(CCCC2(C1CCC3(C2CCC4C3(CCC5C4(CCC5C(C)(C)O)C)C)C)C)C	FALSE	0.1545	94

	1,2,3,3a,4,5,6,7,7a,9,10,11,11b,12,13,13a-hexadecahydrocyclopenta[a]chrysen-3-yl]propan-2-ol				
117290	1-ethynyl-2,2,6-trimethylcyclohexan-1-ol	CC1CCCC(C1(C#C)O)(C)C	FALSE	0.1538	95
578221	(2,3-dimethyl-3-tricyclo[2.2.1.02,6]heptanyl)methanol	CC1(C2CC3C1(C3C2)C)CO	FALSE	0.1538	96
1268143	(1R,2R,5S)-2,6,6-trimethylbicyclo[3.1.1]heptan-2-ol	CC1(C2CCC(C1C2)(C)O)C	FALSE	0.1455	97
10128	2,6,6-trimethylbicyclo[3.1.1]heptan-2-ol	CC1(C2CCC(C1C2)(C)O)C	FALSE	0.1455	98
6428289	(1R,2S,5S)-2,6,6-trimethylbicyclo[3.1.1]heptan-2-ol	CC1(C2CCC(C1C2)(C)O)C	FALSE	0.1455	99
86619	2-methoxy-6-(2,3,3-trimethyl-2-bicyclo[2.2.1]heptanyl)cyclohexan-1-ol	CC1(C2CCC(C2)C1(C)C3CCCC(C3O)OC)C	FALSE	0.1447	100
221170	2-hydroperoxy-2,6,6-trimethylbicyclo[3.1.1]heptane	CC1(C2CCC(C1C2)(C)OO)C	FALSE	0.1379	101
10353	2-(4-methylcyclohexyl)propan-2-ol	CC1CCC(CC1)C(C)(C)O	FALSE	0.1333	102
368926	2,6,6,9-tetramethyltricyclo[5.4.0.02,9]undecane-8,11-diol	CC1(CCCC2(C3C1C(C2(CC3O)C)O)C)C	FALSE	0.1299	103
21119328	(1S,2R,7R,8R,9S,11R)-2,6,6,9-tetramethyltricyclo[5.4.0.02,9]undecane-8,11-diol	CC1(CCCC2(C3C1C(C2(CC3O)C)O)C)C	FALSE	0.1299	104
379930	1,5,5-trimethylbicyclo[2.2.1]heptan-2-ol	CC1(CC2(CC1CC2O)C)C	FALSE	0.1273	105

165258	(1R,4aR,7R,8aR)-7-(2-hydroxypropan-2-yl)-1,4a-dimethyl-2,3,4,5,6,7,8,8a-octahydronaphthalen-1-ol	CC12CCCC(C1CC(CC2)C(C)(C)O)(C)O	FALSE	0.127	106
52940854	(1R,4aR,8aR)-7-(2-hydroxypropan-2-yl)-1,4a-dimethyl-2,3,4,5,6,7,8,8a-octahydronaphthalen-1-ol	CC12CCCC(C1CC(CC2)C(C)(C)O)(C)O	FALSE	0.127	107
4655876	7-(2-hydroxypropan-2-yl)-1,4a-dimethyl-2,3,4,5,6,7,8,8a-octahydronaphthalen-1-ol	CC12CCCC(C1CC(CC2)C(C)(C)O)(C)O	FALSE	0.127	108
85157952	7-(2-hydroxypropan-2-yl)-1,4a-dimethyl-2,3,4,5,6,7,8,8a-octahydro-1H-naphthalen-2-ol	CC1C(CCC2(C1CC(CC2)C(C)(C)O)C)O	FALSE	0.127	109
44237348	(1S,9S,13R,14R)-5,5,9,14-tetramethyltetracyclo[11.2.1.01,10.04,9]hexadecan-14-ol	CC1(CCCC2(C1CCC34C2CCC(C3)C(C4)(C)O)C)C	FALSE	0.1176	110
623309	5,5,9,14-tetramethyltetracyclo[11.2.1.01,10.04,9]hexadecan-14-ol	CC1(CCCC2(C1CCC34C2CCC(C3)C(C4)(C)O)C)C	FALSE	0.1176	111
21593607	(1S,4R,9R,10R,13R,14R)-5,5,9,14-tetramethyltetracyclo[11.2.1.01,10.04,9]hexadecan-14-ol	CC1(CCCC2(C1CCC34C2CCC(C3)C(C4)(C)O)C)C	FALSE	0.1176	112
12112093	(1S,4R,9R,10R,13R,14S)-14-(hydroxymethyl)-5,5,9-trimethyltetracyclo[11.2.1.01,10.04,9]hexadecan-14-ol	CC1(CCCC2(C1CCC34C2CCC(C3)C(C4)(CO)O)C)C	FALSE	0.1136	113

26196128	(1S,4S,6R,9S,10R,13R,14R)-14-(hydroxymethyl)-5,5,9-trimethyltetracyclo[11.2.1.01,10.04,9]hexadecane-6,14-diol	CC1(C2CCC34CC(CCC3C2(CCC1O)C)C(C4)(CO)O)C	FALSE	0.1087	114
22476645	1-methyl-3-(2-methylpropyl)cyclohexan-1-ol	CC(C)CC1CCCC(C1)(C)O	FALSE	0.1087	115
596186	4,4,8-trimethyltricyclo[6.3.1.01,5]dodecane-2,9-diol	CC1(CC(C23C1CCC(C2)(C(CC3)O)C)O)C	FALSE	0.1081	116
76319362	(1S,2S,8R,9R)-4,4,8-trimethyltricyclo[6.3.1.01,5]dodecane-2,9-diol	CC1(CC(C23C1CCC(C2)(C(CC3)O)C)O)C	FALSE	0.1081	117
15599878	(1S,2S,5S,8R,9R)-4,4,8-trimethyltricyclo[6.3.1.01,5]dodecane-2,9-diol	CC1(CC(C23C1CCC(C2)(C(CC3)O)C)O)C	FALSE	0.1081	118
85998	2-(3,3-dimethyl-2-bicyclo[2.2.1]heptanyl)ethanol	CC1(C2CCC(C2)C1CCO)C	FALSE	0.1053	119
106672	1-(3,3-dimethyl-2-bicyclo[2.2.1]heptanyl)ethanol	CC(C1C2CCC(C2)C1(C)C)O	FALSE	0.1034	120
99843	3,3-dimethylbicyclo[2.2.1]heptane-2-carboxylic acid	CC1(C2CCC(C2)C1C(=O)O)C	FALSE	0.1034	121
22326187	1-(2,2,3,6-tetramethylcyclohexyl)hexan-3-ol	CCCC(CCC1C(CCC(C1(C)C)C)C)O	FALSE	0.1034	122
137834	2-tert-butyl-5-methylcyclohexan-1-ol	CC1CCC(C(C1)O)C(C)(C)C	FALSE	0.102	123

61125	4,4,8-trimethyltricyclo[6.3.1.02,5]dodecan-1-ol	CC1(CC2C1CCC3(CCCC2(C3)O)C)C	FALSE	0.1014	124
11746218	(1R,2S,5R,8S)-4,4,8-trimethyltricyclo[6.3.1.02,5]dodecan-1-ol	CC1(CC2C1CCC3(CCCC2(C3)O)C)C	FALSE	0.1014	125
11020495	(1aS,4aR,5R,7aS,7bR)-3,3,5,7b-tetramethyl-1,1a,2,4,5,6,7,7a-octahydrocyclopropa[h]azulen-4a-ol	CC1CCC2C1(CC(CC3C2(C3)C)(C)C)O	FALSE	0.0986	126
11057730	(1S,3R,4R,6S,8S,9R,10R,13R,14R,16R)-5,5,9,14-tetramethyltetracyclo[11.2.1.01,10.04,8]hexadecane-3,4,6,9,14,16-hexol	CC1(C(CC2C1(C(CC34CC(C(C3O)CCC4C2(C)O)(C)O)O)O)O)C	FALSE	0.0943	127
3511	5,5,9,14-tetramethyltetracyclo[11.2.1.01,10.04,8]hexadecane-3,4,6,9,14,16-hexol	CC1(C(CC2C1(C(CC34CC(C(C3O)CCC4C2(C)O)(C)O)O)O)O)C	FALSE	0.0943	128
207666	(3R,4R,6R,8S,9R,10R,14R,16S)-5,5,9,14-tetramethyltetracyclo[11.2.1.01,10.04,8]hexadecane-3,4,6,9,14,16-hexol	CC1(C(CC2C1(C(CC34CC(C(C3O)CCC4C2(C)O)(C)O)O)O)O)C	FALSE	0.0943	129
1.29E+08	(1R,5R,7S,8R)-2,6,6,8-tetramethyltricyclo[5.3.1.01,5]undecan-8-ol	CC1CCC2C13CCC(C(C3)C2(C)C)(C)O	FALSE	0.0933	130
522667	2,6,6,8-tetramethyltricyclo[5.3.1.01,5]undecan-8-ol	CC1CCC2C13CCC(C(C3)C2(C)C)(C)O	FALSE	0.0933	131

6708665	(2R,5S,8R)-2,6,6,8-tetramethyltricyclo[5.3.1.01,5]undecan-8-ol	CC1CCC2C13CCC(C(C3)C2(C)C)(C)O	FALSE	0.0933	132
65575	(1S,2R,5S,7R,8R)-2,6,6,8-tetramethyltricyclo[5.3.1.01,5]undecan-8-ol	CC1CCC2C13CCC(C(C3)C2(C)C)(C)O	FALSE	0.0933	133
1.46E+08	(1S,8R)-2,6,6,8-tetramethyltricyclo[5.3.1.01,5]undecan-8-ol	CC1CCC2C13CCC(C(C3)C2(C)C)(C)O	FALSE	0.0933	134
12302603	(1R,2R,5S,7R,8R)-2,6,6,8-tetramethyltricyclo[5.3.1.01,5]undecan-8-ol	CC1CCC2C13CCC(C(C3)C2(C)C)(C)O	FALSE	0.0933	135
1.35E+08	(2R,7R,8R)-2,6,6,8-tetramethyltricyclo[5.3.1.01,5]undecan-8-ol	CC1CCC2C13CCC(C(C3)C2(C)C)(C)O	FALSE	0.0933	136
6432709	(8S)-2,6,6,8-tetramethyltricyclo[5.3.1.01,5]undecan-8-ol	CC1CCC2C13CCC(C(C3)C2(C)C)(C)O	FALSE	0.0933	137
6713078	(1S,2R,5S,7R,8S)-2,6,6,8-tetramethyltricyclo[5.3.1.01,5]undecan-8-ol	CC1CCC2C13CCC(C(C3)C2(C)C)(C)O	FALSE	0.0933	138
7285502	(1R,2R,5R,7S,8R)-2,6,6,8-tetramethyltricyclo[5.3.1.01,5]undecan-8-ol	CC1CCC2C13CCC(C(C3)C2(C)C)(C)O	FALSE	0.0933	139
108424	1-(2,2,6-trimethylcyclohexyl)pentan-3-ol	CCC(CCC1C(CCCC1(C)C)C)O	FALSE	0.0926	140

116699	1-(2,2,6-trimethylcyclohexyl)hexan-3-ol	CCCC(CCC1C(CCCC1(C)C)C)O	FALSE	0.0909	141
11085796	(1S,2R,5S,7R,8R)-8-methoxy-2,6,6,8-tetramethyltricyclo[5.3.1.01,5]undecane	CC1CCC2C13CCC(C(C3)C2(C)C)(C)OC	FALSE	0.0897	142
24758199	8-methoxy-2,6,6,8-tetramethyltricyclo[5.3.1.01,5]undecane	CC1CCC2C13CCC(C(C3)C2(C)C)(C)OC	FALSE	0.0897	143
88288	(1S,2R,5S,7R,8S)-8-methoxy-2,6,6,8-tetramethyltricyclo[5.3.1.01,5]undecane	CC1CCC2C13CCC(C(C3)C2(C)C)(C)OC	FALSE	0.0897	144
433104	5,5,9,14-tetramethyltetracyclo[11.2.1.01,10.04,8]hexadecane-3,4,6,14,16-pentol	CC1C2CCC3C(C2(CC(C4(C1CC(C4(C)C)O)O)O)CC3(C)O)O	FALSE	0.0874	145
171535	5,5,9,14-tetramethyltetracyclo[11.2.1.01,10.04,8]hexadecane-2,3,4,6,9,14,16-heptol	CC1(C(CC2C1(C(C(C34CC(C(C3O)CCC4C2(C)O)(C)O)O)O)O)O)C	FALSE	0.0804	146
44559353	(1R,2S,3R,4R,6S,8S,9R,10R,13R,14R,16R)-5,5,9,14-tetramethyltetracyclo[11.2.1.01,10.04,8]hexadecane-2,3,4,6,9,14,16-heptol	CC1(C(CC2C1(C(C(C34CC(C(C3O)CCC4C2(C)O)(C)O)O)O)O)O)C	FALSE	0.0804	147
107272	4-(2,2,6-trimethylcyclohexyl)butan-2-ol	CC1CCCC(C1CCC(C)O)(C)C	FALSE	0.0755	148
92030006	2,2,6,6,7,8,8-heptamethyl-3,3a,4,5,5a,7,8a,8b-octahydrocyclopenta[g][1]benzofuran	CC1C(C2CCC3CC(OC3C2C1(C)C)(C)C)(C)C	FALSE	0.075	149
12315274	2,3-dimethylbicyclo[2.2.1]heptan-2-ol	CC1C2CCC(C2)C1(C)O	FALSE	0.0714	150
14841556	(3S,4S,5S,8S,9S,10R,13R,14S,17R)-4,10,13-trimethyl-17-[(2R)-6-methylheptan-2-yl]-	CC1C2CCC3C4CCC(C4(CCC3C2(CCC1O)C)C)C(C)CCCC(C)C	FALSE	0.07	151

	2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol				
103005	3-(5,5,6-trimethyl-2-bicyclo[2.2.1]heptanyl)cyclohexan-1-ol	CC1C2CC(C1(C)C)CC2C3CCCC(C3)O	FALSE	0.0694	152
106673	4-(5,5,6-trimethyl-2-bicyclo[2.2.1]heptanyl)cyclohexan-1-ol	CC1C2CC(C1(C)C)CC2C3CCC(CC3)O	FALSE	0.0694	153
109188	3-(5,5-dimethyl-6-methylidene-2-bicyclo[2.2.1]heptanyl)cyclohexan-1-ol	CC1(C2CC(C(C2)C1=C)C3CCCC(C3)O)C	FALSE	0.0694	154
526611	5,5-dimethyl-6-methylidenebicyclo[2.2.1]heptan-2-ol	CC1(C2CC(C1=C)C(C2)O)C	FALSE	0.0678	155
99038	2,6,6-trimethylbicyclo[3.1.1]heptan-3-ol	CC1C2CC(C2(C)C)CC1O	FALSE	0.0678	156
7271803	(1S,2R,3R,5R)-2,6,6-trimethylbicyclo[3.1.1]heptan-3-ol	CC1C2CC(C2(C)C)CC1O	FALSE	0.0678	157
90350	(1S,2S,3S,5R)-2,6,6-trimethylbicyclo[3.1.1]heptan-3-ol	CC1C2CC(C2(C)C)CC1O	FALSE	0.0678	158
10524983	(1R,2R,3R,5S)-2,6,6-trimethylbicyclo[3.1.1]heptan-3-ol	CC1C2CC(C2(C)C)CC1O	FALSE	0.0678	159
10944069	(1aR,3aS,7S,7aS,7bR)-1,1,3a,7-tetramethyl-1a,2,3,4,5,6,7a,7b-octahydrocyclopropa[a]naphthalen-7-ol	CC1(C2C1C3C(CCCC3(C)O)(CC2)C)C	FALSE	0.0676	160
521185	1,4,4,7-tetramethyltricyclo[5.3.1.02,6]undecan-11-ol	CC1(CC2C(C1)C3(CCCC2(C3O)C)C)C	FALSE	0.0658	161

14038123	(1S,2R,6S,7R)-1,4,4,7-tetramethyltricyclo[5.3.1.02,6]undecan-11-ol	CC1(CC2C(C1)C3(CCCC2(C3O)C)C)C	FALSE	0.0658	162
164822	1,2-dimethylcyclohexan-1-ol	CC1CCCCC1(C)O	FALSE	0.0652	163
11581815	(1S,3R,4R,6R,7R,8S,9R,10R,13R,14R,16R)-5,5,9,14-tetramethyltetracyclo[11.2.1.01,10.04,8]hexadecane-3,4,6,7,9,14,16-heptol	CC1(C(C(C2C1(C(CC34CC(C(C3O)CCC4C2(C)O)(C)O)O)O)O)O)C	FALSE	0.0619	164
11042078	(1R,3aR,4S,7aR)-1-[(2S)-1-hydroxypropan-2-yl]-7a-methyl-1,2,3,3a,4,5,6,7-octahydroinden-4-ol	CC(CO)C1CCC2C1(CCCC2O)C	FALSE	0.0615	165
174845	1-(4-ethyl-2-bicyclo[2.2.1]heptanyl)cyclohexan-1-ol	CCC12CCC(C1)C(C2)C3(CCCCC3)O	FALSE	0.0571	166
110745	1,1,4,7-tetramethyl-2,3,4,5,6,7,7a,7b-octahydro-1aH-cyclopropa[h]azulen-4a-ol	CC1CCC2(C1C3C(C3(C)C)CCC2C)O	FALSE	0.0526	167
572865	(3,3,7-trimethyl-8-tricyclo[5.4.0.02,9]undecanyl)methanol	CC1(CCCC2(C3C1C(C2CO)CC3)C)C	FALSE	0.0526	168
108425	3-methyl-4-(2,2,6-trimethylcyclohexyl)butan-2-ol	CC1CCCC(C1CC(C)C(C)O)(C)C	FALSE	0.0526	169
12311096	[(1R,2S,7S,8S,9S)-3,3,7-trimethyl-8-tricyclo[5.4.0.02,9]undecanyl]methanol	CC1(CCCC2(C3C1C(C2CO)CC3)C)C	FALSE	0.0526	170
536562	3,7,7-trimethylbicyclo[4.1.0]heptan-2-ol	CC1CCC2C(C1O)C2(C)C	FALSE	0.0508	171
6326181	(1R,2R,5S)-2-methyl-5-propan-2-ylbicyclo[3.1.0]hexan-2-ol	CC(C)C12CCC(C1C2)(C)O	FALSE	0.05	172

11228920	(1S,2S,5R)-2-methyl-5-propan-2-ylbicyclo[3.1.0]hexan-2-ol	CC(C)C12CCC(C1C2)(C)O	FALSE	0.05	173
57357974	2,6,6,7,8,8-hexamethyl-3,3a,4,5,5a,7,8a,8b-octahydro-2H-cyclopenta[g][1]benzofuran	CC1CC2CCC3C(C2O1)C(C(C3(C)C)C)(C)C	FALSE	0.05	174
62367	2-methyl-5-propan-2-ylbicyclo[3.1.0]hexan-2-ol	CC(C)C12CCC(C1C2)(C)O	FALSE	0.05	175
16218817	2-methyl-5-propan-2-ylbicyclo[3.1.0]hexan-2-ol;hydrate	CC(C)C12CCC(C1C2)(C)O.O	FALSE	0.05	176
67159878	(1R,5S)-2-methyl-5-propan-2-ylbicyclo[3.1.0]hexan-2-ol	CC(C)C12CCC(C1C2)(C)O	FALSE	0.05	177
20055523	(1R,2S,5S)-2-methyl-5-propan-2-ylbicyclo[3.1.0]hexan-2-ol	CC(C)C12CCC(C1C2)(C)O	FALSE	0.05	178
11744854	(1S,2R,5R)-2-methyl-5-propan-2-ylbicyclo[3.1.0]hexan-2-ol	CC(C)C12CCC(C1C2)(C)O	FALSE	0.05	179
1.18E+08	1-ethyl-2-(3-methylbutyl)cyclopentan-1-ol	CCC1(CCCC1CCC(C)C)O	FALSE	0.037	180
564727	4,7,7-trimethylbicyclo[4.1.0]heptan-2-ol	CC1CC2C(C2(C)C)C(C1)O	FALSE	0.0339	181
73828281	1,5-dimethyl-4-(2-methylprop-1-enyl)-1,2,3,4,5,6,7,7a-octahydroinden-3a-ol	CC1CCC2C(CCC2(C1C=C(C)C)O)C	FALSE	0.0294	182
11976203	4,10-dimethyl-7-propan-2-yltricyclo[4.4.0.01,5]decan-4-ol	CC1CCC(C2C13C2C(CC3)(C)O)C(C)C	FALSE	0.0253	183
11276107	(1R,4S,5R,6R,7S,10R)-4,10-dimethyl-7-propan-2-yltricyclo[4.4.0.01,5]decan-4-ol	CC1CCC(C2C13C2C(CC3)(C)O)C(C)C	FALSE	0.0253	184

12304217	(1S,4S,5S,6S,7R,10S)-4,10-dimethyl-7-propan-2-yltricyclo[4.4.0.01,5]decan-4-ol	CC1CCC(C2C13C2C(CC3)(C)O)C(C)C	FALSE	0.0253	185
46187190	(1R,4S,5R,6R,7S,10S)-4,10-dimethyl-7-propan-2-yltricyclo[4.4.0.01,5]decan-4-ol	CC1CCC(C2C13C2C(CC3)(C)O)C(C)C	FALSE	0.0253	186
21308	2-bicyclo[2.2.1]heptanylmethanol	C1CC2CC1CC2CO	FALSE	0.0189	187
98106	4-tricyclo[5.2.1.02,6]decanylmethanol	C1CC2CC1C3C2CC(C3)CO	FALSE	0.0154	188
56842534	1-ethyl-3-methoxytricyclo[2.2.1.02,6]heptane	CCC12CC3CC1C2C3OC	FALSE	0.0143	189
160138	[8-(hydroxymethyl)-3-tricyclo[5.2.1.02,6]decanyl]methanol	C1CC2C3CC(C2C1CO)CC3CO	FALSE	0.0141	190
109415	spiro[oxolane-2,8'-tricyclo[5.2.1.02,6]decane]	C1CC2C(C1)C3CC2CC34CCCO4	FALSE	0.0132	191
297765	3-(1,1,1,3,3,3-hexafluoro-2-hydroxypropan-2-yl)bicyclo[2.2.1]heptan-2-ol	C1CC2CC1C(C2O)C(C(F)(F)F)(C(F)(F)F)O	FALSE	0.0127	192
12304603	(1S,3S,4S,5R)-4-methyl-1-propan-2-ylbicyclo[3.1.0]hexan-3-ol	CC1C2CC2(CC1O)C(C)C	FALSE	0	193
12304610	(1S,3S,4R,5R)-4-methyl-1-propan-2-ylbicyclo[3.1.0]hexan-3-ol	CC1C2CC2(CC1O)C(C)C	FALSE	0	194
10550	4-methyl-1-propan-2-ylbicyclo[3.1.0]hexan-3-ol	CC1C2CC2(CC1O)C(C)C	FALSE	0	195
19792960	2-ethyl-5-methoxybicyclo[2.2.1]heptane	CCC1CC2CC1CC2OC	FALSE	0	196

12304609	(1R,3R,4S,5S)-4-methyl-1-propan-2-ylbicyclo[3.1.0]hexan-3-ol	CC1C2CC2(CC1O)C(C)C	FALSE	0	197
95606	tricyclo[5.2.1.02,6]decan-8-ol	C1CC2C(C1)C3CC2CC3O	FALSE	0	198
98091	[8-(hydroxymethyl)-4-tricyclo[5.2.1.02,6]decanyl]methanol	C1C(CC2C1C3CC(C2C3)CO)CO	FALSE	0	199
3034320	(1R,3R)-4-methyl-1-propan-2-ylbicyclo[3.1.0]hexan-3-ol	CC1C2CC2(CC1O)C(C)C	FALSE	0	200

Table S3. Main Parameters from Modified Randles Circuit Fitting for All EIS Samp

Sample	Double Layer CPE ($F \cdot s^{n-1}$)	CPE Exponent for Double Layer	Charge Transfer Resistance (Ω)	R^2 Re(Z)	R^2 Im(Z)
GCE	1.322×10^{-6}	0.893	411.31	0.99994	0.99958
GCE_Au	2.884×10^{-6}	0.849	245.82	0.99996	0.99976
MIP	1.940×10^{-6}	0.865	15,466.63	0.99994	0.99992
MIP_W	3.439×10^{-6}	0.868	8,108.07	0.99993	0.99994
MIP_R	3.847×10^{-6}	0.883	12,616.94	0.99977	0.99990

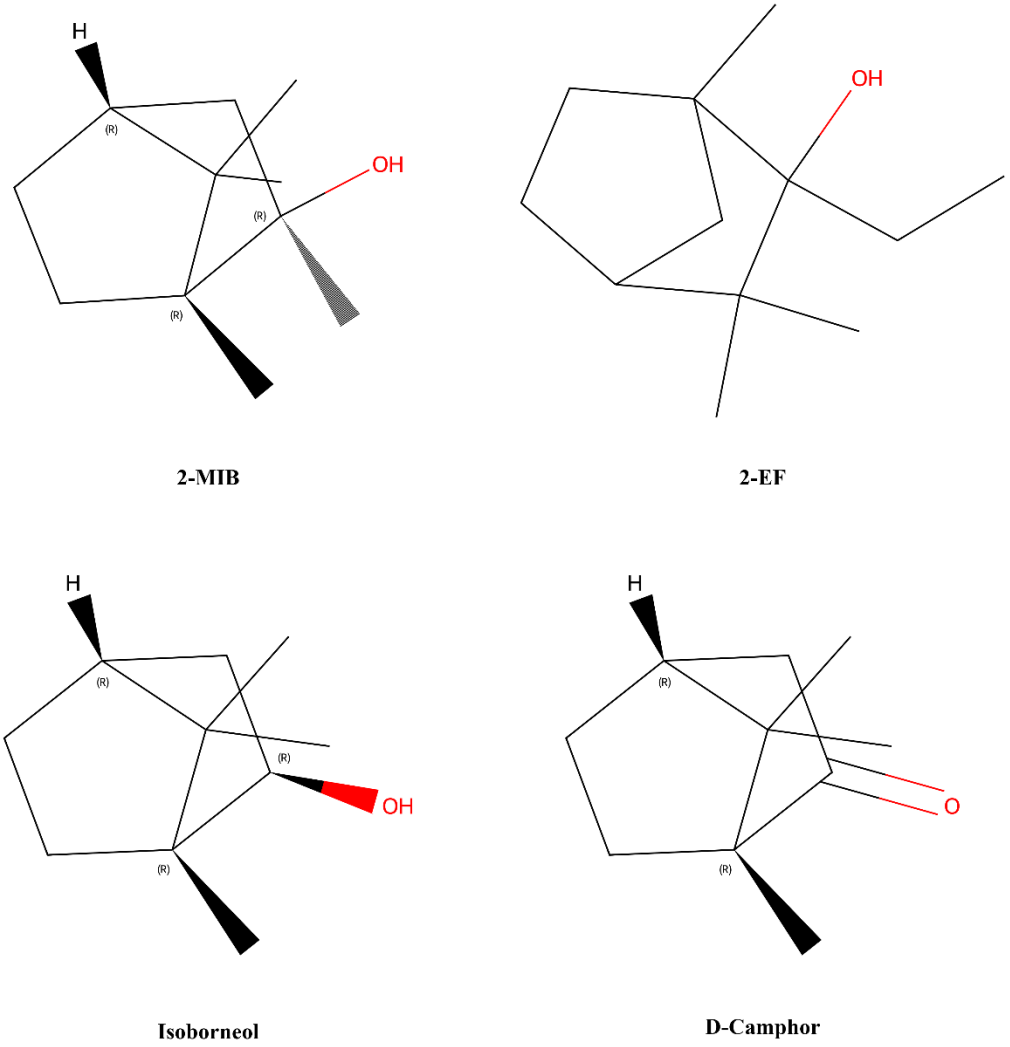

Fig. S3. Chemical structures of 2-methylisoborneol (2-MIB) and its structural analogs evaluated for dummy template selection.

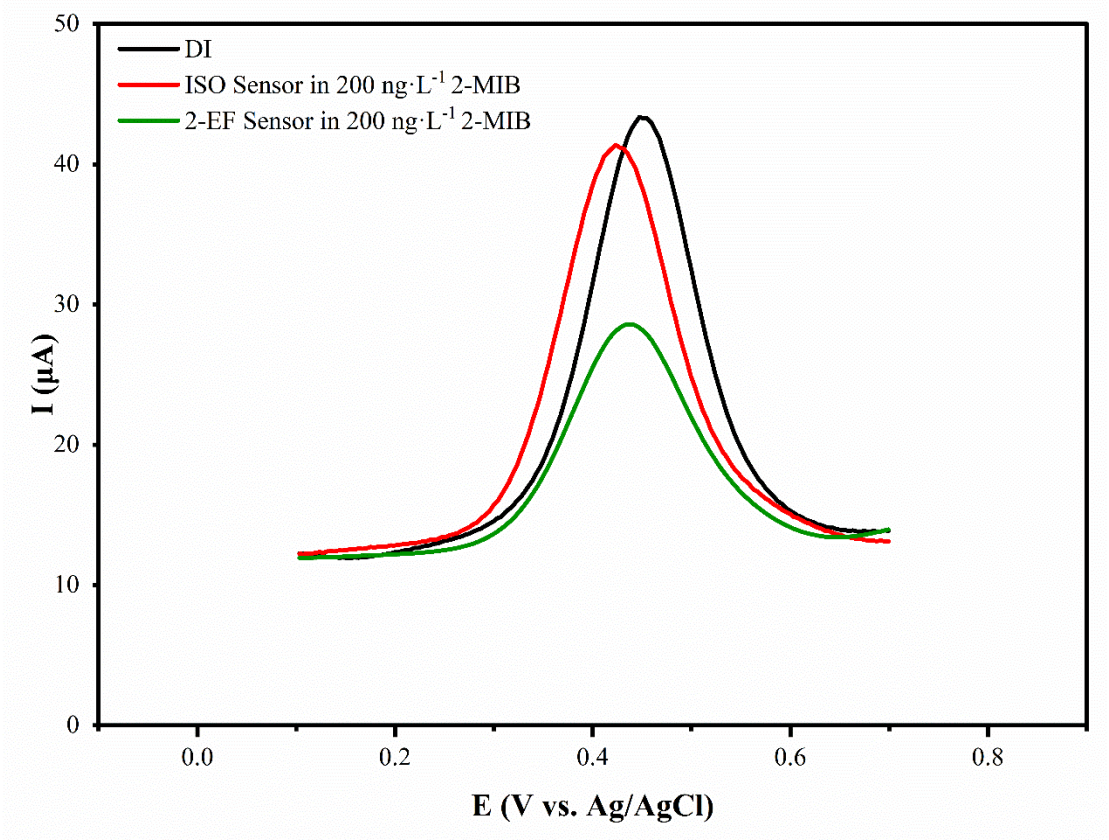

Fig. S4. Interference Evaluation of Structurally Related Compounds on the IHEN Sensor

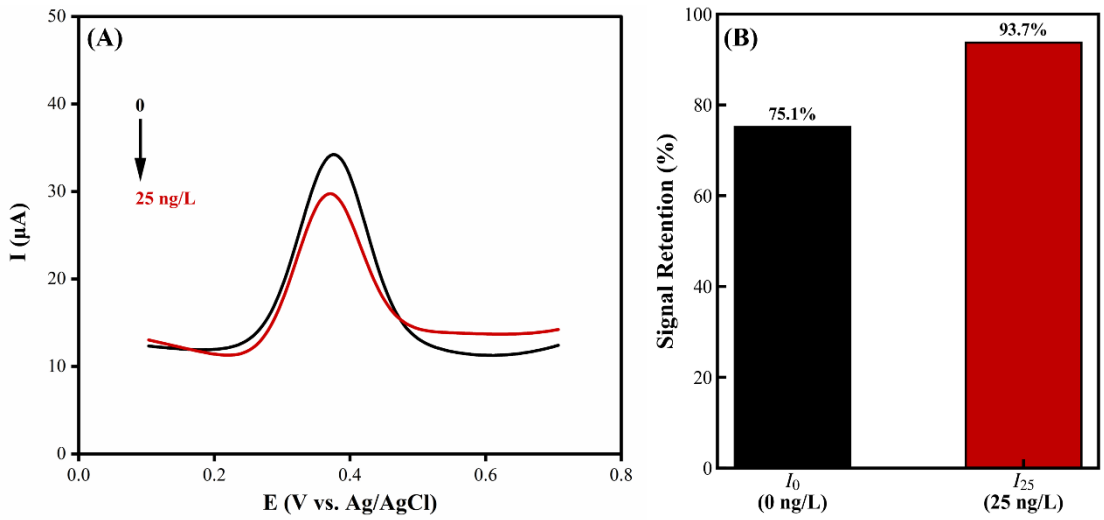

Figure S5. Long-term stability evaluation of the AuNP-MIP/GCE sensor. (A) Square wave voltammograms (SWV) recorded in DI water containing 0 ng/L and 25 ng/L 2-MIB after 7 days of storage at 4 °C. (B) Signal retention (%) of the peak currents at 0 ng/L (I_0) and 25 ng/L (I_{25}) after 7-day storage, normalized to the corresponding fresh-sensor values.

Section S1. Cartesian coordinates of input and optimized structures used in the DFT calculations

S1.1 o-PD monomer (GFN2-xTB)

16

o-Phenylenediamine (o-PD) monomer — GFN2-xTB optimized

C	1.53684638	-0.75365675	1.13135483
C	1.27218251	0.54844948	1.51098941
C	0.25038586	1.24651626	0.89179167
C	-0.53017748	0.66383880	-0.09842175
C	-0.26894261	-0.66652971	-0.47619759
C	0.77215505	-1.34768197	0.14336670
N	-1.07173316	-1.33169849	-1.39841304
N	-1.59938098	1.37600856	-0.64904038
H	2.33660328	-1.30892211	1.59776103
H	1.86030806	1.02647276	2.27971232
H	0.04280301	2.26818838	1.18006279
H	0.97300723	-2.36706516	-0.15638698
H	-0.64610719	-2.14571618	-1.81358847
H	-1.56940285	-0.76040365	-2.06210824
H	-1.80190143	1.18510032	-1.61929761
H	-1.55664666	2.36709745	-0.46158569

S1.2 2-MIB monomer (GFN2-xTB)

35

2-Methylisoborneol (2-MIB) monomer — GFN2-xTB optimized

C	-2.12743493	-0.07702872	1.28705626
C	-1.17269824	-0.23139280	0.09371390
C	0.05677698	-1.12955280	0.41105621
C	0.64849792	-0.68648200	1.75753294
C	1.27700753	0.67957130	1.41190010
C	1.01822658	0.81211683	-0.09751250
C	-0.48758602	1.11711048	-0.33347599
O	-0.75843400	1.35801101	-1.71086646
C	-0.96726805	2.38008891	0.39578971
C	1.16883109	-0.65355459	-0.55818436
C	0.95862434	-0.90840756	-2.05334061
C	2.54940090	-1.26466115	-0.27190832
C	-2.05203249	-0.84334354	-1.00656930
H	-1.71768129	0.49140787	2.11360275
H	-3.03587487	0.42273628	0.95951935
H	-2.39923429	-1.06436125	1.65583824
H	-0.18295386	-2.19153397	0.36956592
H	-0.09640788	-0.61796245	2.54396010
H	1.39255594	-1.40320074	2.10266406
H	0.83897723	1.49279616	1.98451289

H	2.34838613	0.69656295	1.61088114
H	1.67122535	1.53487891	-0.59023259
H	-0.30255706	2.16741987	-1.96382679
H	-0.94993403	2.30715136	1.47524774
H	-0.33367307	3.21788846	0.10268974
H	-1.98643285	2.59529551	0.08267543
H	0.15825733	-0.31625539	-2.47336330
H	1.87032007	-0.65379437	-2.59228823
H	0.75679919	-1.96481044	-2.22115007
H	2.87433457	-1.20022699	0.75826320
H	2.53669648	-2.31626357	-0.55309320
H	3.29805418	-0.76243497	-0.88254633
H	-2.74766304	-0.09653792	-1.37928407
H	-2.62123620	-1.66967320	-0.58498468
H	-1.48386864	-1.22155548	-1.84384187

S1.3 2-EF monomer (GFN2-xTB)

35

2-Ethylfenchol (2-EF) monomer — GFN2-xTB optimized

C	3.17605500	1.17745800	0.12073500
C	2.19306300	0.36070600	-0.70996900
C	1.06749400	-0.24285000	0.14116200
C	0.04096200	0.77488700	0.74975400
C	-0.55656100	0.05404300	1.99205200
C	-1.49153600	-0.99569400	1.36092900
C	-1.29373800	-0.75953400	-0.15658000
C	0.12906800	-1.26839600	-0.57182400
C	0.45026200	-2.71201200	-0.17727800
O	0.26518300	-1.22652700	-1.99025600
C	-1.16826800	0.79375100	-0.22464800
C	-2.40396000	1.56351400	0.30680100
C	-0.91441800	1.40595000	-1.61113700
H	3.99798100	1.52985600	-0.51086700
H	2.69631700	2.05517800	0.56284000
H	3.60622000	0.57514800	0.92720600
H	1.81653900	1.00067700	-1.50876600
H	2.74945600	-0.45293500	-1.19116400
H	1.57275800	-0.74933600	0.97571900
H	0.45925800	1.75298700	0.99453300
H	-1.11419300	0.74656200	2.63109800
H	0.20846500	-0.41054300	2.62302400
H	-2.53114900	-0.81968100	1.65761300
H	-1.25447300	-2.01012400	1.68858200
H	-2.09987600	-1.16460500	-0.77425100

H	0.54392800	-2.85406800	0.90267800
H	1.39623700	-3.02990100	-0.63174300
H	-0.32103400	-3.39421500	-0.55197200
H	-0.42643600	-1.79265400	-2.37347700
H	-2.73488300	1.28946600	1.30963000
H	-2.19709300	2.63995800	0.33826000
H	-3.26338200	1.40596900	-0.35563600
H	-0.08933100	0.98671700	-2.17667900
H	-0.70717900	2.47900700	-1.52101000
H	-1.80173400	1.29124300	-2.24535900

S1.4 Isoborneol monomer (GFN2-xTB)

29

Isoborneol (IB) monomer — GFN2-xTB optimized

C	-2.16930532	-0.43946936	-0.01117902
C	-0.71980338	-0.26457105	0.44193282
C	0.17199129	-1.48107959	0.12290989
C	0.17449327	-1.51497309	-1.41160251
C	0.11755342	-0.02288981	-1.79157597
C	0.12950169	0.69629012	-0.43023384
C	1.56424931	0.48539192	0.11802439
C	1.55802000	-0.99787793	0.55656138
O	1.86098464	1.38026138	1.17092637
C	-0.29084573	2.15020181	-0.48860301
C	-0.76382045	0.10245376	1.92563583
H	-2.71131425	0.49599237	0.10604030
H	-2.26344991	-0.75762506	-1.04237748
H	-2.65103415	-1.18683230	0.61628537
H	-0.12582837	-2.42248032	0.58321520
H	1.07421155	-1.99914269	-1.79155642
H	-0.68100792	-2.06702319	-1.79900305
H	-0.78994608	0.22257802	-2.34167385
H	0.96379142	0.27899885	-2.40887672
H	2.29215187	0.65303419	-0.69014697
H	1.67924700	-1.06929857	1.63754466
H	2.35671698	-1.57180505	0.08564669
H	2.76028410	1.20947121	1.46794064
H	-0.21081987	2.59869001	0.49698617
H	0.35782059	2.69835459	-1.16871238
H	-1.31553120	2.23622329	-0.84161553
H	-1.00924644	-0.77736470	2.51756083
H	-1.53413426	0.85088502	2.09614663
H	0.17507220	0.51360614	2.27380157

S1.5 D-camphor monomer (GFN2-xTB)

27

D-Camphor monomer — GFN2-xTB optimized

C	1.61536101	-1.16934309	-0.49154749
C	0.74362788	-0.14362116	0.22795840
C	0.65082390	1.21769846	-0.49621346
C	-0.05510519	0.85876703	-1.80980544
C	-1.07614935	-0.20512676	-1.36699884
C	-0.77779110	-0.40905444	0.13867334
C	-1.33635004	0.86691429	0.75170541
O	-2.34634447	0.98564510	1.39092618
C	-0.37724468	1.97308284	0.34765786
C	-1.33220897	-1.68942365	0.72425649
C	1.24493211	-0.03743226	1.66975466
H	2.64535527	-0.81841993	-0.51323021
H	1.59274440	-2.11617940	0.04342113
H	1.29670084	-1.35241339	-1.51143885
H	1.59368267	1.74629689	-0.62881572
H	0.64836820	0.46540025	-2.54236642
H	-0.53570600	1.73038536	-2.25334585
H	-0.95081264	-1.14521779	-1.90341081
H	-2.10541816	0.12299029	-1.51512118
H	-0.90221288	2.75289625	-0.20510520
H	0.05650770	2.43989232	1.23154524
H	-2.41661046	-1.69307872	0.63638043
H	-1.07891788	-1.76439922	1.77907317
H	-0.93470528	-2.55694993	0.20182459
H	0.54868759	0.49650214	2.31028746
H	1.38408572	-1.03111574	2.08970974
H	2.20469882	0.47530626	1.69422637

S1.6 2-EF + o-PD complex (B3LYP-D3(BJ)/def2-SVP)

51

2-EF + oPD complex, B3LYP-D3(BJ)/def2-SVP optimized, E = -888.18711976 Ha

C	2.585048	-1.005237	-1.006057
C	1.587613	-0.380765	-1.987291
C	0.123006	-0.033368	-1.609315
C	-0.086290	1.136849	-0.535218
C	-0.957977	0.429438	0.551033
C	-2.393786	0.199816	0.052505
C	-2.198380	-0.875816	-1.048519
C	-0.683903	-1.227764	-0.975658
C	-0.409827	-1.007964	0.527367
C	-0.396146	-2.600204	-1.571020

C	1.201563	1.644357	0.134562
C	-0.766801	2.364805	-1.153578
O	-0.476912	0.382449	-2.837622
H	2.889394	-0.325553	-0.201016
H	3.497588	-1.279871	-1.559331
H	2.207087	-1.924711	-0.538502
H	2.027235	0.541563	-2.401356
H	1.514050	-1.063368	-2.847479
H	-0.906515	0.948606	1.519650
H	-3.011791	-0.184717	0.877558
H	-2.878173	1.113371	-0.315441
H	-2.476839	-0.516018	-2.046281
H	-2.791696	-1.779561	-0.836534
H	0.649525	-1.087913	0.802869
H	-0.986279	-1.697251	1.164823
H	0.650924	-2.911329	-1.453731
H	-0.626746	-2.612771	-2.649607
H	-1.028195	-3.363542	-1.090443
H	0.960734	2.527146	0.748503
H	1.958140	1.954158	-0.601921
H	1.656429	0.903024	0.804551
H	-1.074036	3.060401	-0.354169
H	-1.643747	2.111099	-1.758137
H	-0.065413	2.900823	-1.812903
H	-0.538546	-0.382177	-3.452175
C	2.912017	-2.627310	-5.901704
C	3.667012	-1.455596	-5.977124
C	3.054717	-0.215265	-5.776322
C	1.683440	-0.115160	-5.500747
C	0.917067	-1.306794	-5.462046
C	1.538695	-2.543363	-5.647279
N	-0.463485	-1.197517	-5.167689
N	1.031019	1.104336	-5.296411
H	3.381687	-3.601277	-6.044206
H	4.738952	-1.503066	-6.181603
H	3.649965	0.700860	-5.810431
H	0.932892	-3.453314	-5.604119
H	-0.982236	-2.047482	-5.372176
H	-0.880509	-0.403543	-5.659007
H	0.467332	1.115795	-4.438610
H	1.660167	1.901852	-5.312122

S1.7 2-MIB + o-PD complex (B3LYP-D3(BJ)/def2-SVP)

48

2-MIB + oPD complex, B3LYP-D3(BJ)/def2-SVP optimized, E = -848.90343936 Ha

C	-2.525518757121	0.062044558128	0.298527339365
C	-1.075439522278	-0.447158783929	0.352968181842
C	-0.558150565579	-0.688274188095	1.799488388575
C	-0.599144680971	0.726929259252	2.423242170010
C	-0.278100970314	1.650718555088	1.214210153511
C	0.014989118462	0.657086398931	0.064156856968
C	1.364587527348	-0.085702922272	0.422173431329
C	0.919805953991	-1.043957239489	1.566415715094
C	2.516363694626	0.831969025220	0.842658993359
O	1.815577862425	-0.877055682346	-0.679220905664
C	0.010782138998	1.286598550668	-1.317057059429
C	-1.024392207219	-1.686902332963	-0.553179715854
H	-2.737102817242	0.903814271256	0.969177331704
H	-3.213435108780	-0.754135906907	0.571836691151
H	-2.787728822686	0.376613694157	-0.724439138618
H	-1.111791573170	-1.446402057784	2.374465288438
H	-1.583158385815	0.953942882263	2.858599273305
H	0.137174135415	0.824451592646	3.235897030297
H	0.554943264459	2.340136759885	1.399679124042
H	-1.141286107954	2.277624527034	0.949290549402
H	1.044563109822	-2.083353087747	1.235066862571
H	1.526211006864	-0.911184198545	2.475100661791
H	2.315780728674	1.356030371603	1.785865032264
H	2.738084210665	1.585931576817	0.070558543001
H	3.423992797281	0.227350430973	0.982666972253
H	2.296830627916	-0.310871078492	-1.323840151458
H	-0.945986717220	1.794355781468	-1.516893624065
H	0.165676540799	0.530994378873	-2.101035349549
H	0.807966016925	2.042656852971	-1.413878956546
H	-1.398422592392	-1.434545905449	-1.559164699028
H	-0.019638957867	-2.097578688366	-0.680108301439
H	-1.686803981977	-2.470230416164	-0.148253317246
C	7.121412645449	0.392972151576	0.075220772296
C	6.734549929015	1.483518231490	-0.703900731543
C	5.630044176946	1.365169680071	-1.554216155255
C	4.905607893265	0.174235398602	-1.627295303082
C	5.266750177110	-0.925065475687	-0.807066015133
C	6.388598104411	-0.796093214696	0.023140274672
N	4.513655824332	-2.100503121416	-0.901312227370
N	3.770618576721	0.032451585153	-2.461627236638
H	7.987564713634	0.465798749489	0.736805870550
H	7.291227694096	2.422028137062	-0.662082812506
H	5.330976425280	2.207365229486	-2.185261548070

H	6.676391765834	-1.644742639662	0.650494917269
H	4.828165457436	-2.826474222462	-0.264693968609
H	3.507362395831	-1.935867766931	-0.778825929917
H	3.743621591781	-0.898722632165	-2.883515949812
H	3.722320629799	0.742344926471	-3.188387865867

S1.8 Isoborneol + o-PD complex (B3LYP-D3(BJ)/def2-SVP)

45

IB + oPD complex, B3LYP-D3(BJ)/def2-SVP optimized, E = -809.60717998 Ha

C	-1.956066	-0.169638	0.452067
C	-0.429781	-0.130759	0.609802
C	0.275220	-1.433895	0.130467
C	-0.061480	-1.477288	-1.374938
C	-0.046109	0.028397	-1.772220
C	0.310676	0.761638	-0.453010
C	1.809569	0.421638	-0.211802
C	1.765374	-1.068461	0.244968
O	2.404950	1.273094	0.747790
C	0.006292	2.247975	-0.462934
C	-0.134343	0.242621	2.070878
H	-2.390957	0.822661	0.650783
H	-2.297434	-0.488479	-0.541732
H	-2.388531	-0.867715	1.188489
H	-0.005647	-2.345142	0.681838
H	0.679662	-2.069864	-1.934020
H	-1.042843	-1.937593	-1.561055
H	-1.027689	0.361480	-2.142204
H	0.684927	0.255136	-2.564086
H	2.355161	0.527341	-1.170212
H	2.123665	-1.133776	1.282602
H	2.402343	-1.723683	-0.370283
H	3.374778	1.091572	0.759563
H	0.277736	2.715801	0.494534
H	0.573972	2.758383	-1.257183
H	-1.063970	2.429357	-0.648847
H	-0.401172	-0.596808	2.736350
H	-0.750343	1.104773	2.373522
H	0.911498	0.514658	2.242777
C	6.781313	2.085157	3.997202
C	6.112940	3.243942	4.393628
C	5.130540	3.801492	3.569930
C	4.797252	3.223200	2.335669
C	5.506238	2.065676	1.927008
C	6.476009	1.505226	2.760978

N 5.164740 1.492759 0.672008
N 3.851262 3.775495 1.469101
H 7.544709 1.635634 4.635725
H 6.344775 3.713779 5.351028
H 4.594259 4.701116 3.890040
H 7.007939 0.609171 2.427342
H 5.834722 0.788581 0.370039
H 5.081480 2.213700 -0.044444
H 3.193464 3.095789 1.074668
H 3.346778 4.558602 1.869890

S1.9 D-camphor + o-PD complex (B3LYP-D3(BJ)/def2-SVP)

43
D-Camphor + oPD complex, B3LYP-D3(BJ)/def2-SVP optimized, E = -808.40484290 Ha
C 1.605841 -1.387035 -1.113627
C 0.972961 -0.179044 -0.413659
C 0.838932 1.081315 -1.325721
C -0.111627 0.598903 -2.440898
C -1.111702 -0.309008 -1.666467
C -0.576154 -0.311801 -0.198236
C -0.911046 1.097042 0.284025
O -1.769447 1.388302 1.089465
C 0.030553 2.049545 -0.445312
C -1.112322 -1.407530 0.694188
C 1.746803 0.072394 0.888065
H 2.658937 -1.169522 -1.353902
H 1.594436 -2.263371 -0.446791
H 1.102697 -1.673505 -2.046667
H 1.793889 1.490274 -1.683801
H 0.425800 0.036899 -3.216521
H -0.607592 1.442144 -2.941084
H -1.124541 -1.338662 -2.053044
H -2.149654 0.056877 -1.711158
H -0.543303 2.804199 -1.005079
H 0.614664 2.599811 0.306169
H -2.199360 -1.294650 0.824076
H -0.658263 -1.356712 1.694989
H -0.914003 -2.404786 0.273289
H -1.286509 1.202836 4.366385
H 1.826844 -0.856440 1.474508
H 2.771501 0.409820 0.665235
C 2.673180 1.348395 4.596753
C 3.273638 2.346247 3.827980
C 2.475048 3.220008 3.082121

C	1.081325	3.106222	3.086597
C	0.467178	2.067038	3.836876
C	1.280442	1.213117	4.590611
N	-0.931075	1.991992	3.837561
N	0.263770	3.937367	2.315530
H	3.283690	0.664915	5.192398
H	4.360701	2.459673	3.816562
H	2.939138	4.014774	2.489667
H	0.806306	0.420615	5.176296
H	1.291268	0.825712	1.543850
H	-1.338903	1.977522	2.899187
H	0.681671	4.826385	2.062330
H	-0.667669	4.055286	2.705430

Table S4. Key parameters used in the MD simulations

Parameters	**Value**
Software	GROMACS
Force field (solute)	GAFF2
Water model	TIP3P
Box size	40 × 40 × 40 Å
Template molecules	1 (2-EF or 2-MIB)
o-PD molecules	10
NH_4^+ ions	4
CH_3COO^- ions	4
CH_3COOH molecules	2
Water molecules	~2000
Integrator	leap-frog
Time step	1 fs
Thermostat	V-rescale
τ	0.1 ps
Tref	298.15 K
Electrostatics	PME
rcoulomb	1.2 nm
vdW cutoff	1.2 nm
Constraints	LINCS
Energy minimization	steepest descent
NVT equilibration	100 ps
NPT equilibration	100 ps
Production run	10 ns (NVT)
Analysis window	last 8 ns