

## Supporting Information

### **Role of MoO<sub>x</sub>/Ni(111) Interfacial Sites in Direct Deoxygenation of Phenol toward Benzene**

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### Microkinetic parameter analysis:

The reaction rate constant was calculated according to the transition state theory, and the forward rate constant ( $k_f$ ) was calculated using the formula:

$$k_f = \frac{k_B T}{h} \frac{q_{TS,vib}}{q_{IS,vib}} e^{-\frac{E_a}{k_B T}} \quad (S1)$$

where  $k_B$ ,  $T$  and  $h$  are Boltzmann constant, reaction temperature and the Planck's constant, respectively.  $E_a$  is the ZPE-corrected activation barrier for the forward reaction obtained from DFT calculations, and  $q_{IS,vib}$  and  $q_{TS,vib}$  are the vibrational partition functions for the initial state and the transition state, respectively. The vibration partition function can be calculated according to the formula:

$$q_{vib} = \prod_i \frac{1}{1 - e^{-h\nu_i/k_B T}} \quad (S2)$$

where  $\nu_i$  is the vibrational frequency for each vibrational mode of the adsorbed intermediate,  $i$  runs to  $N - 1$  and  $N$  for the transition state and initial state, respectively. The reverse rate constant ( $k_r$ ) was estimated similarly.

The desorption rate constant ( $k_{des}$ ) can be obtained from the adsorption rate constant ( $k_{ad}$ ) and adsorption equilibrium constant ( $K_{eq}$ ):

$$k_{des} = \frac{k_{ad}}{K_{eq}} \quad (S3)$$

where  $k_{ad}$  was calculated based on the collision theory. For a non-activated adsorption process,  $k_{ad}$  was calculated according to:<sup>54-56</sup>

$$k_{ad} = \frac{S\sigma}{\sqrt{2\pi mk_B T}} \quad (S4)$$

where  $m$ ,  $k_B$  and  $T$  represent the molecular mass, Boltzmann constant and temperature, respectively. The sticking coefficient  $\sigma$  was assumed to be 1.0 for the adsorbing species.  $S$  is the area of each adsorption site. The equilibrium constant ( $K_{eq}$ ) was calculated using:

$$K_{eq} = \frac{(q_{vib})_{A^*}}{(q_{vib}q_{rot}q_{tra})_{A(g)}} e^{-\frac{\Delta E_{ads}}{RT}} \quad (S5)$$

where  $q_{rot}$  and  $q_{tra}$  are the rotation partition function and the translation partition function, respectively. They were calculated using the following equations:

$$q_{rot} = \frac{\sqrt{\pi}}{\sigma} \left(\frac{8\pi^2 k_B T}{h^2}\right)^{\frac{3}{2}} \sqrt{I_x I_y I_z} \quad (S6)$$

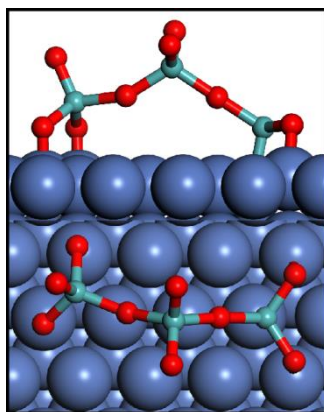
$$q_{tra} = \left(\frac{2\pi m k_B T}{h^2}\right)^{\frac{3}{2}} V \quad (S7)$$

where  $\sigma$  is the symmetry coefficient of the desorbed species.  $I_x$  is the moment of inertia of the desorbed species taking the  $x$ -axis direction as the direction of the rotation axis, and  $I_y$  and  $I_z$  are similar.  $V$  is the volume of the translational space of the desorbed species.

**Table S1.** Adsorption energy of phenol and benzene on Ni(111) and Mo<sub>3</sub>O<sub>5</sub>/Ni(111) (with or without vdw)

	Ni(111)	Mo <sub>3</sub> O <sub>5</sub> /Ni(111)
Phenol(with vdw <sup>a</sup> )/eV	-1.83	-1.86
Phenol(without vdw)/eV	-0.72	-0.67
Benzene(with vdw <sup>a</sup> )/eV	-1.91	-2.06
Benzene(without vdw)/eV	-0.86	-0.83

<sup>a</sup> Calculated using VDW correction through DFT-D3 method of Grimme with zero-damping function.



**Fig. S1** The structure of the chain Mo<sub>3</sub>O<sub>9</sub>/Ni(111).

**Table S2.** Core level shift of Mo 3d in Mo<sub>3</sub>O<sub>5</sub>/Ni(111) and Mo<sub>3</sub>O<sub>7</sub>/Ni(111) relative to Mo<sub>3</sub>O<sub>9</sub>/Ni(111) and the comparison of experimental values.

Calculation <sup>a</sup>			Experiment <sup>b</sup>	
Species of Mo		E <sub>CLS</sub> <sup>c</sup> /eV	The valence of Mo	E <sub>CLS</sub> <sup>c</sup> /eV
Mo <sub>3</sub> O <sub>9</sub> /Ni(111)	Mo	0	Mo <sup>6+</sup>	0
Mo <sub>3</sub> O <sub>5</sub> /Ni(111)	Mo <sub>ov</sub>	-4.90	Mo <sup>3+</sup>	-5.50
	Mo <sub>1</sub> <sup>d</sup>	-3.87		
	Mo <sub>2</sub> <sup>e</sup>	-3.84	Mo <sup>4+</sup>	-3.30
Mo <sub>3</sub> O <sub>7</sub> /Ni(111)	Mo <sub>ov</sub>	-4.67	Mo <sup>5+</sup>	-1.40
	Mo <sub>1</sub> <sup>d</sup>	-3.20		
	Mo <sub>2</sub> <sup>e</sup>	-3.08		

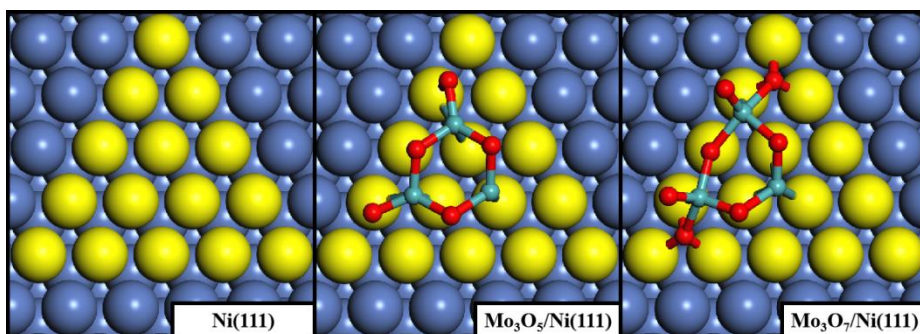
a Using the final-state approximation to calculate core energies E<sub>core</sub>.

b From the ref. 24 in the paper.<sup>24</sup>

c Core level shift relative to Mo<sub>3</sub>O<sub>9</sub>/Ni(111) or Mo<sup>6+</sup>.

d The first Mo counterclockwise from Mo<sub>ov</sub>.

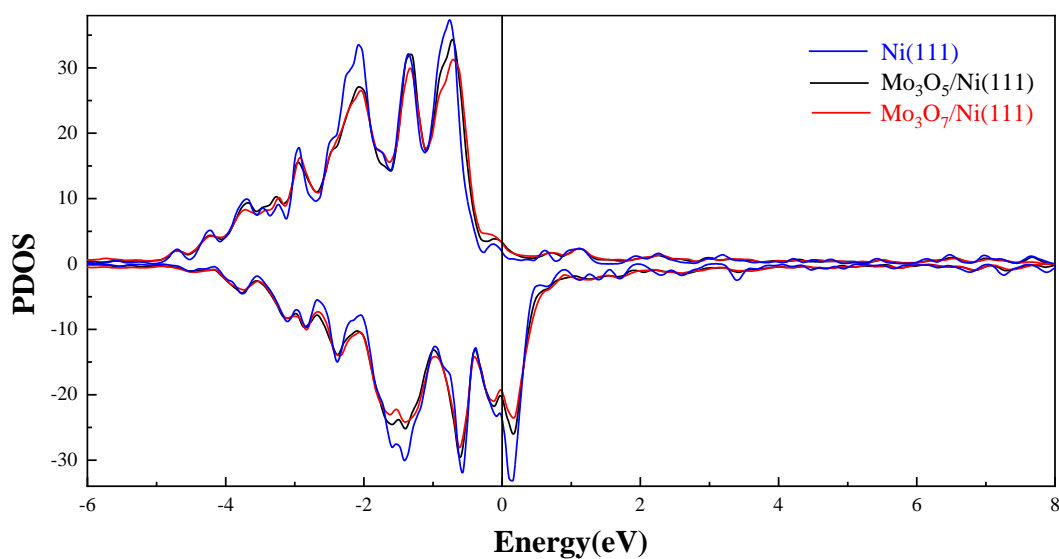
e The first Mo clockwise from Mo<sub>ov</sub>.



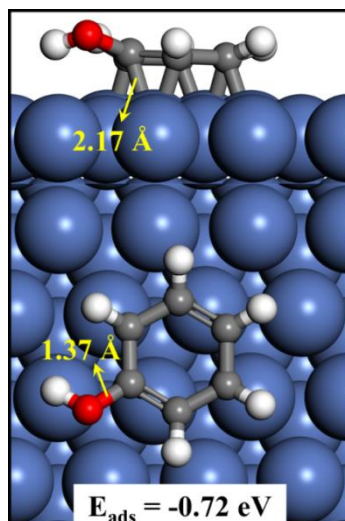
**Fig. S2** The area of the PDOS (yellow atoms for the atoms involved in integration).

**Table S3.** The d band centers and the peak area of the both spin up and down of Ni atoms near the cluster.

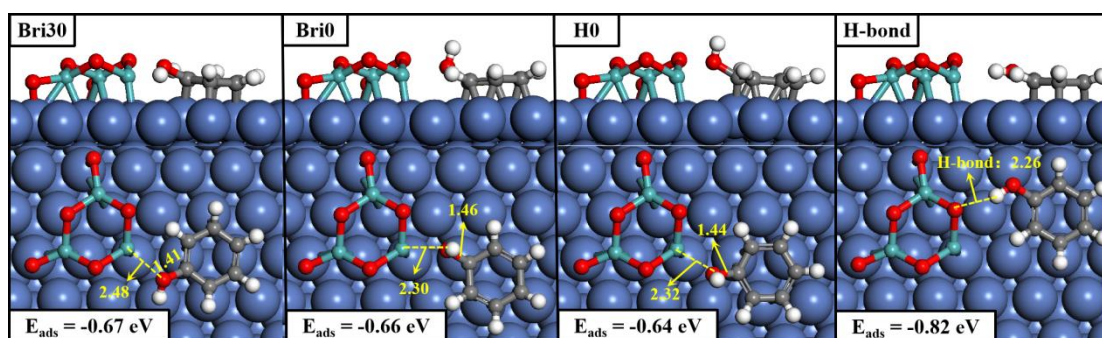
Surface	d-band center (eV)		Area of peak	
	Spin up	Spin down	Spin up	Spin down
Ni(111)	-1.51	-0.78	72.88	72.57
Mo <sub>3</sub> O <sub>5</sub> /Ni(111)	-1.55	-0.93	72.80	72.47
Mo <sub>3</sub> O <sub>7</sub> /Ni(111)	-1.58	-0.98	72.80	72.54



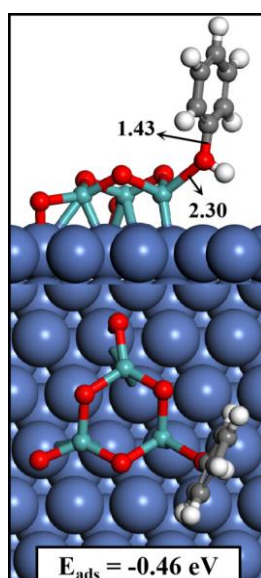
**Fig. S3** PDOS diagram of Ni atoms on the three surfaces.



**Fig. S4** The stable adsorption configurations of phenol on Ni(111).

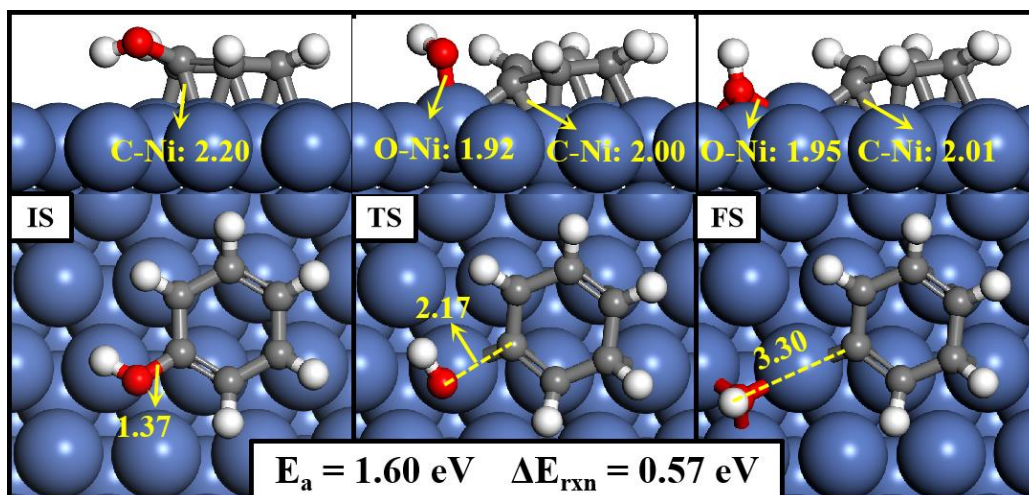


**Fig. S5** Different adsorption configurations and adsorption energy of phenol at the  $\text{Mo}_3\text{O}_5/\text{Ni}(111)$  interface. The yellow number represents the bond length or the distance between two atoms, in Å.

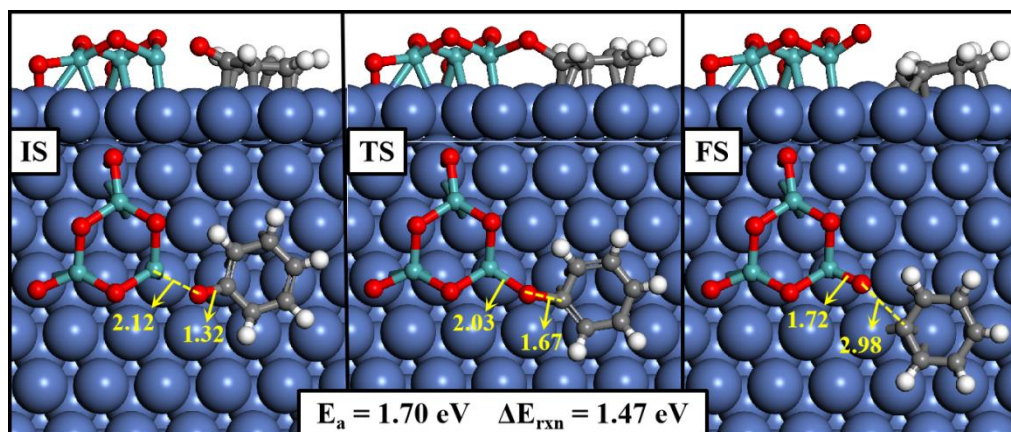


**Fig. S6** Vertical adsorption configuration of phenol on  $\text{Mo}_{\text{ov}}$  at the  $\text{Mo}_3\text{O}_5/\text{Ni}(111)$  interface. The number represents the bond length, in Å.





**Fig. S7** Structures of initial state (IS), transition state (TS), and final state (FS) in direct deoxygenation of phenol on 3-layer 6×6 Ni(111) surface.



**Fig. S8** Structures of initial state (IS), transition state (TS), and final state (FS) in direct deoxygenation of phenoxy on Ni(111).

## References

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cluster\_mo3o5

1.0000000000000000

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0.0000000000000000	0.0000000000000000	19.0690994262999993

Ni	Mo	O
108	3	5

Selective dynamics

Direct

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0.0001654001751909	0.0000357894398695	0.2114707332823471	T	T	T
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cluster\_mo3o7

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Ni Mo O

100 3 7

Selective dynamics

Direct

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0.0011112854268789	0.1991862324486652	0.2998170089913387	T	T	T
0.2015896709794234	0.2027453900356946	0.9991513435129207	F	F	F
0.3343773157108885	0.2687954475866547	0.0977086281376529	F	F	F
0.2678913151532182	0.3347421447941554	0.1963049052483870	T	T	T
0.1973232251780642	0.1990831658853556	0.2987277760910239	T	T	T
0.4013155826643455	0.2022547464251687	0.9993764926289188	F	F	F
0.5340667262433314	0.2683896779573516	0.0976302463589036	F	F	F
0.4673300873753409	0.3346216922582457	0.1957294369405154	T	T	T
0.4001260402604264	0.1968906388292275	0.2950533480822863	T	T	T
0.6015971111550229	0.2027168810697901	0.9999399012514587	F	F	F
0.7345721731620642	0.2684769072000321	0.0976624567897417	F	F	F
0.6665691318269884	0.3331368771406221	0.1963895321711371	T	T	T

0.5988604361024851	0.1978196561543424	0.3051126863540018	T	T	T
0.8012371763334656	0.2022155106078429	0.9991569313064304	F	F	F
0.9344922480870608	0.2690052660049531	0.0976451810961407	F	F	F
0.8676436250189549	0.3348045373194535	0.1953633797436641	T	T	T
0.7976819109942641	0.1967606885134721	0.2933591629482235	T	T	T
0.0006424211689477	0.4020766796969681	0.9991198054930450	F	F	F
0.1343487903935454	0.4689749961674252	0.0964301214325900	F	F	F
0.0665207221448468	0.5337205174670686	0.1968247626888757	T	T	T
0.0030965845107504	0.4065808941313189	0.2975994904163792	T	T	T
0.2011195229829639	0.4018827147913129	0.9984748440733071	F	F	F
0.3346863201013974	0.4688285944891106	0.0964815842940467	F	F	F
0.2675542953856533	0.5349733030942435	0.1945258622324738	T	T	T
0.2030781881076814	0.4054386374217038	0.2919182592869955	T	T	T
0.4017857549495218	0.4019370300789973	0.9992964473094332	F	F	F
0.5342976520741516	0.4681301116132559	0.0974756262936651	F	F	F
0.4672572514808648	0.5334907415511649	0.1969237560639423	T	T	T
0.4041185228593013	0.4062356935330216	0.2971464239387071	T	T	T
0.6013224183380927	0.4024131998278691	0.9993988338859978	F	F	F
0.7344559297954518	0.4687162149379276	0.0973789326590548	F	F	F
0.6680703924390063	0.5356038540528711	0.1949386126421937	T	T	T
0.6041283091560121	0.4040782785573117	0.2921994294923687	T	T	T
0.8016893996145171	0.4025224490277850	0.9993696473864873	F	F	F
0.9341502515244287	0.4683251265964188	0.0973753723281519	F	F	F
0.8675840815782839	0.5355162835668100	0.1947374830369749	T	T	T
0.8004412771301538	0.4036267322024642	0.2916553616355753	T	T	T
0.0012912825346021	0.6022000057600323	0.9977908902587913	F	F	F
0.1343768598952266	0.6680866662621625	0.0950295313187937	F	F	F
0.0672835305347961	0.7344869201129263	0.1944444137802710	T	T	T
0.0006281015993310	0.6030075772421275	0.2939203070455343	T	T	T
0.2006957624980714	0.6010415435028378	0.9966859051203372	F	F	F
0.3337687126591433	0.6674162186486257	0.0944221031660533	F	F	F
0.2671691392031109	0.7342653389816415	0.1940653644876510	T	T	T
0.2016639713229278	0.6030848660824489	0.2928754050208713	T	T	T
0.4008269554586334	0.6009393316036196	0.9968516560055605	F	F	F
0.5338910773035721	0.6680844749319377	0.0952076918844327	F	F	F
0.4672538524234722	0.7343132146214929	0.1940618509225222	T	T	T
0.4017825899320076	0.6030590359952088	0.2929103821251505	T	T	T
0.6013278413011562	0.6019485087268706	0.9979514065206772	F	F	F
0.7340751507812371	0.6683253118015955	0.0958886038159292	F	F	F
0.6672495376514380	0.7344922479342032	0.1945804982517303	T	T	T
0.6029259991672572	0.6031033463587253	0.2941775028270820	T	T	T
0.8009465729592620	0.6013925893888796	0.9980453576992829	F	F	F
0.9345537288335208	0.6686207347045183	0.0956451480535137	F	F	F
0.8677444920612409	0.7353646076765010	0.1939795202709967	T	T	T

0.8024217785956695	0.6037791923961038	0.2945917897475083	T	T	T
0.0013588973653853	0.8020118193581922	0.9973972989082114	F	F	F
0.1345277936195188	0.8684519742502701	0.0953639449683976	F	F	F
0.0670311666419841	0.9347845243480813	0.1943380139175517	T	T	T
-0.0000776575580458	0.8004677634957336	0.2929299681788431	T	T	T
0.2017573349696562	0.8021767531556989	0.9975543897272843	F	F	F
0.3343228129954312	0.8681198832608956	0.0957973310232845	F	F	F
0.2675076407292941	0.9347400243348242	0.1944610789445971	T	T	T
0.2000075376706563	0.7998429653452512	0.2927052770279490	T	T	T
0.4012821234673751	0.8020315704945986	0.9977785034166757	F	F	F
0.5340544904112434	0.8682042775104009	0.0958031397484689	F	F	F
0.4674930197706682	0.9347158152214697	0.1949863610103131	T	T	T
0.4002814773638633	0.8000817794956396	0.2926859530558070	T	T	T
0.6007331633507746	0.8018332447500640	0.9976327988332301	F	F	F
0.7340231019997674	0.8683545597100633	0.0954941355844525	F	F	F
0.6673152405584203	0.9348318516831258	0.1945383692126482	T	T	T
0.6000187534595330	0.7999179393363884	0.2927804621891981	T	T	T
0.8009778239988563	0.8017598646696982	0.9975281489910302	F	F	F
0.9349310270731195	0.8698092836506675	0.0946045884108528	F	F	F
0.8677881123531701	0.9346816791748105	0.1943621905621906	T	T	T
0.8007252007627755	0.8002286342969922	0.2929314032414712	T	T	T
0.7700174025463563	0.2299995537181602	0.4118019650442509	T	T	T
0.7407390064973910	0.4839069232695761	0.4043358116139052	T	T	T
0.4633139407039689	0.2464605087782585	0.4137226757897341	T	T	T
0.8302751816562309	0.4050998800939634	0.4404388448296202	T	T	T
0.5668743576032811	0.4063853353052138	0.4473161312802297	T	T	T
0.5878430786140489	0.1951546711375391	0.4022286862530030	T	T	T
0.7607158889180318	0.1305332957504065	0.4722442423614213	T	T	T
0.3637696819895737	0.1435310164262931	0.4706630386804524	T	T	T
0.3426807005841712	0.2725020557695363	0.3610360495509480	T	T	T
0.9292793783954475	0.2730822604237346	0.3592962629073142	T	T	T

phenol\_ddo\_mo3o5\_is

1.0000000000000000

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-7.4753999709999999 12.9477725567000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.0690994262999993

Ni Mo O C H  
108 3 6 6 6

Selective dynamics

Direct

0.1111000029999971	0.0555500019999968	0.0018000000000029	F	F	F
0.0555500019999968	0.1111100019999967	0.1066899969999966	F	F	F
0.0008698180414642	0.0012445050811809	0.2115006806722301	T	T	T
0.2777900099999968	0.0555699989999994	0.0017899999999997	F	F	F
0.2222100050000009	0.1111000029999971	0.1066799979999971	F	F	F
0.1644304601543619	0.9995446260249755	0.2125012048763722	T	T	T
0.4444499909999990	0.0555500019999968	0.0018000000000029	F	F	F
0.3889000120000006	0.1111100019999967	0.1066799979999971	F	F	F
0.3289656308665944	0.9962039060235216	0.2148308214042502	T	T	T
0.6111000180000019	0.0555500019999968	0.0018000000000029	F	F	F
0.5555499789999985	0.1111100019999967	0.1067000030000003	F	F	F
0.4988985970829812	0.9992236235618350	0.2124141266425954	T	T	T
0.7777900099999968	0.0555699989999994	0.0017899999999997	F	F	F
0.7222099900000032	0.1111000029999971	0.1066799979999971	F	F	F
0.6683779994910464	0.9991137656082241	0.2178212232961949	T	T	T
0.9444500210000015	0.0555500019999968	0.0018000000000029	F	F	F
0.8888900279999987	0.1111000029999971	0.1066799979999971	F	F	F
0.8363608564705970	0.0018991736638451	0.2109607675332691	T	T	T
0.1111199999999997	0.2222400010000030	0.0018099999999990	F	F	F
0.0555599999999998	0.2777799959999996	0.1067200009999993	F	F	F
0.0013283524955559	0.1680824478439662	0.2115740369733771	T	T	T
0.2777900099999968	0.2222200040000004	0.0017899999999997	F	F	F
0.2222200040000004	0.2777799959999996	0.1067200009999993	F	F	F
0.1668983441482747	0.1680605809116332	0.2114350635131837	T	T	T
0.4444299939999965	0.2222100050000009	0.0017899999999997	F	F	F
0.3889000120000006	0.2777900099999968	0.1066799979999971	F	F	F
0.3332713479261094	0.1689657249917977	0.2109334449347473	T	T	T
0.6111199859999985	0.2222400010000030	0.0018099999999990	F	F	F
0.5555599930000028	0.2777799959999996	0.1067200009999993	F	F	F
0.5015617577928239	0.1677873580861398	0.2161507892243229	T	T	T
0.7777799959999996	0.2222100050000009	0.0017899999999997	F	F	F
0.7222200040000004	0.2777799959999996	0.1067200009999993	F	F	F
0.6670112931347609	0.1684209447340878	0.2133103950362511	T	T	T
0.9444299940000036	0.2222100050000009	0.0017899999999997	F	F	F
0.8888999819999981	0.2777900099999968	0.1066799979999971	F	F	F

0.8359149179994150	0.1692802964662150	0.2112006255213364	T	T	T
0.1111199999999997	0.3888800140000015	0.0018099999999990	F	F	F
0.0555599999999998	0.4444499909999990	0.1066899969999966	F	F	F
0.0010800377439937	0.3341197043016171	0.2117029687504277	T	T	T
0.2777599989999970	0.3888800140000015	0.0018099999999990	F	F	F
0.2222200040000004	0.4444400069999972	0.1067200009999993	F	F	F
0.1673394881818384	0.3341728895750540	0.2116956828459984	T	T	T
0.4444499909999990	0.3889000120000006	0.0018000000000029	F	F	F
0.3888899800000033	0.4444499909999990	0.1066899969999966	F	F	F
0.3338249204003561	0.3344707282499663	0.2112288370030495	T	T	T
0.6111199859999985	0.3888800140000015	0.0018099999999990	F	F	F
0.5555599930000028	0.4444499909999990	0.1066899969999966	F	F	F
0.4988961239645009	0.3319918858345123	0.2113599825429733	T	T	T
0.7777600289999995	0.3888800140000015	0.0018099999999990	F	F	F
0.7222200040000004	0.4444400069999972	0.1067200009999993	F	F	F
0.6685112719750186	0.3336784947740635	0.2076138949604771	T	T	T
0.9444500210000015	0.3889000120000006	0.0018000000000029	F	F	F
0.8888900279999987	0.4444499909999990	0.1066899969999966	F	F	F
0.8348414638060696	0.3342385058985663	0.2122929252330633	T	T	T
0.1111000029999971	0.5555499789999985	0.0018000000000029	F	F	F
0.0555500019999968	0.6111099720000013	0.1066899969999966	F	F	F
0.0006326604850355	0.5001338339336878	0.2120430932051079	T	T	T
0.2777900099999968	0.5555700059999964	0.0017899999999997	F	F	F
0.2222100050000009	0.6111000180000019	0.1066799979999971	F	F	F
0.1668154519446391	0.5000727857680202	0.2118036169467759	T	T	T
0.4444499909999990	0.5555499789999985	0.0018000000000029	F	F	F
0.3888899800000033	0.6111099720000013	0.1066799979999971	F	F	F
0.3329319688769080	0.5002690754593619	0.2112184263643592	T	T	T
0.6111000180000019	0.5555499789999985	0.0018000000000029	F	F	F
0.5555499789999985	0.6111099720000013	0.1066899969999966	F	F	F
0.5024975858518439	0.5034385174119761	0.2183508782232333	T	T	T
0.7777900099999968	0.5555700059999964	0.0017899999999997	F	F	F
0.7222099900000032	0.6111000180000019	0.1066799979999971	F	F	F
0.6661153744838574	0.4949127564140139	0.2232379216136285	T	T	T
0.9444500210000015	0.5555499789999985	0.0018000000000029	F	F	F
0.8888900279999987	0.6111099720000013	0.1066799979999971	F	F	F
0.8356262282772130	0.4994009302001810	0.2097883224208658	T	T	T
0.1111199999999997	0.7222399710000005	0.0018099999999990	F	F	F
0.0555599999999998	0.7777799959999996	0.1067200009999993	F	F	F
-0.0005538047683830	0.6661473996355629	0.2115349419124707	T	T	T
0.2777900099999968	0.7222099900000032	0.0017899999999997	F	F	F
0.2222200040000004	0.7777799959999996	0.1067200009999993	F	F	F
0.1658446841180110	0.6657767257280774	0.2118221260085429	T	T	T
0.4444299939999965	0.7222200040000004	0.0017899999999997	F	F	F

0.3889000120000006	0.7777900099999968	0.1066799979999971	F	F	F
0.3322017643225770	0.6663412840736119	0.2116133076551523	T	T	T
0.6111199859999985	0.7222399710000005	0.0018099999999990	F	F	F
0.5555599930000028	0.7777799959999996	0.1067200009999993	F	F	F
0.4973673294711748	0.6678918533448840	0.2103398196875772	T	T	T
0.7777799959999996	0.7222200040000004	0.0017899999999997	F	F	F
0.7222200040000004	0.7777799959999996	0.1067200009999993	F	F	F
0.6671097700542344	0.6744318490371618	0.2155792608886498	T	T	T
0.9444299940000036	0.7222099900000032	0.0017899999999997	F	F	F
0.8888999819999981	0.7777900099999968	0.1066799979999971	F	F	F
0.8321421474362704	0.6653785523139616	0.2177639984247765	T	T	T
0.1111199999999997	0.8888800140000015	0.0018099999999990	F	F	F
0.0555500019999968	0.9444400069999972	0.1067000030000003	F	F	F
-0.0001703549770799	0.8331277256789069	0.2109323756544347	T	T	T
0.2777599989999970	0.8888800140000015	0.0018099999999990	F	F	F
0.2222200040000004	0.9444400069999972	0.1067200009999993	F	F	F
0.1638367774419091	0.8300840053991005	0.2108089216384745	T	T	T
0.4444499909999990	0.8888999819999981	0.0018000000000029	F	F	F
0.3888899980000033	0.9444500210000015	0.1066899969999966	F	F	F
0.3322943037682309	0.8313013748608395	0.2109055507326769	T	T	T
0.6111199859999985	0.8888800140000015	0.0018099999999990	F	F	F
0.5555499789999985	0.9444500210000015	0.1066899969999966	F	F	F
0.4979392387037955	0.8327468413366260	0.2108567571681907	T	T	T
0.7777600289999995	0.8888800140000015	0.0018099999999990	F	F	F
0.7222200040000004	0.9444299940000036	0.1067200009999993	F	F	F
0.6665772666961426	0.8365952072042417	0.2088478457169811	T	T	T
0.9444500210000015	0.8888999819999981	0.0018000000000029	F	F	F
0.8888900279999987	0.9444500210000015	0.1067000030000003	F	F	F
0.8354613755453844	0.8366149158757364	0.2109583332234253	T	T	T
0.4241600040000009	0.0939899979999979	0.3321500119999996	F	F	F
0.6340399979999987	0.2950499949999994	0.3346000020000020	T	T	T
0.6458399890000024	0.0929699989999975	0.3316799999999986	F	F	F
0.4902299940000034	0.2273299989999984	0.3746300039999966	T	T	T
0.7098100190000025	0.2269300070000000	0.3737800119999974	T	T	T
0.5026999709999984	0.0292700010000004	0.3626599910000010	F	F	F
0.2870300109999988	0.0092500000000015	0.3105199929999998	F	F	F
0.7002000210000006	0.0093900000000033	0.3194699880000016	F	F	F
0.7571018862075157	0.4791743740709848	0.3600759579316062	T	T	T
0.6222195471229885	0.6605654038450010	0.3184163779288383	T	T	T
0.5569114497670378	0.5493115860166407	0.3208041786121690	T	T	T
0.6073189801620228	0.4884115980818709	0.3266423201727663	T	T	T
0.7171329874433816	0.5366105211241420	0.3281397693084094	T	T	T
0.7838613244815317	0.6469379305739323	0.3208251349616368	T	T	T
0.7327376791907158	0.7078874087314299	0.3165047285178410	T	T	T



0.5885212971086449	0.7079259436289562	0.3337274371003679	T	T	T
0.4800500330022920	0.5173619943241041	0.3442623084674525	T	T	T
0.5604624044497502	0.4114869160042033	0.3499383785768228	T	T	T
0.7786539255467314	0.7896877295973472	0.3308092667935827	T	T	T
0.8255263588580862	0.5001379956252792	0.3389568536983728	T	T	T
0.8589113501479892	0.6815070226155127	0.3472358547086414	T	T	T

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0.0000000000000000 0.0000000000000000 19.0690994262999993

Ni Mo O C H

108 3 6 6 6

Selective dynamics

Direct

0.1111299989999992	0.0556700010000029	0.0018299999999982	F	F	F
0.0556500000000000	0.1113400010000021	0.1067399980000019	F	F	F
0.0005925493160927	0.0015006828524962	0.2110595102195688	T	T	T
0.2777000070000000	0.0556900019999986	0.0017899999999997	F	F	F
0.2222799959999975	0.1113300029999991	0.1067800000000005	F	F	F
0.1653672375708687	0.0005289679963106	0.2124815216889460	T	T	T
0.4441800119999968	0.0555999990000018	0.0016000000000034	F	F	F
0.3888399900000010	0.1111999969999999	0.1067100019999998	F	F	F
0.3288033259435267	0.9958221496567263	0.2147173195464994	T	T	T
0.6107199790000024	0.0554400010000009	0.0012600000000020	F	F	F
0.5552800299999987	0.1109199970000034	0.1063999980000006	F	F	F
0.4986367648798318	0.9985708817543153	0.2117841491549163	T	T	T
0.7774000169999979	0.0552800000000033	0.0010400000000033	F	F	F
0.7218199969999972	0.1105400029999970	0.1060400009999967	F	F	F
0.6677545015601231	0.9973478799412389	0.2165402479783494	T	T	T
0.9442300199999991	0.0552800000000033	0.0011300000000034	F	F	F
0.8884900210000026	0.1103900000000024	0.1059300009999973	F	F	F
0.8351812054576313	0.0005299232546277	0.2101845304353008	T	T	T
0.1111700009999979	0.2222999930000000	0.0018000000000029	F	F	F
0.0556199999999976	0.2779200080000024	0.1066799979999971	F	F	F
0.0001379839944782	0.1674302543339343	0.2113099710504190	T	T	T
0.2778199910000012	0.2223200050000003	0.0018999999999991	F	F	F
0.2223300039999998	0.2779900130000001	0.1067700010000010	F	F	F
0.1660777244553190	0.1676090542865836	0.2115196040415179	T	T	T
0.4443799849999976	0.2222899940000005	0.0018999999999991	F	F	F
0.3890399929999973	0.2779699860000022	0.1068300009999987	F	F	F
0.3330177730745901	0.1686712505859452	0.2110653348804418	T	T	T
0.6109499929999984	0.2222400010000030	0.0016999999999996	F	F	F
0.5556200150000024	0.2777700130000014	0.1068100040000033	F	F	F
0.5021463339995031	0.1677213376725033	0.2166070733774542	T	T	T
0.7774900200000019	0.2220100019999975	0.0013799999999975	F	F	F
0.7220399979999996	0.2774600090000021	0.1064900009999974	F	F	F
0.6663467910157312	0.1674076748379094	0.2124494684034167	T	T	T
0.9440900090000000	0.2218600060000000	0.0011599999999987	F	F	F
0.8886299730000005	0.2771300080000003	0.1061500010000032	F	F	F

0.8348969042547715	0.1686802113681389	0.2105240633645689	T	T	T
0.11110000010000007	0.3888199929999985	0.0016699999999972	F	F	F
0.0554599990000000	0.4444800019999988	0.1065199969999995	F	F	F
0.9995656099466116	0.3339817304580947	0.2113755654645747	T	T	T
0.2777299879999973	0.3888700010000008	0.0017799999999966	F	F	F
0.2222000060000013	0.4445700050000028	0.1065699979999977	F	F	F
0.1659379634748997	0.3336584824045899	0.2117558451181043	T	T	T
0.4444899860000007	0.3889000120000006	0.00189000000000031	F	F	F
0.3889600039999976	0.4446099999999973	0.1066500020000021	F	F	F
0.3319695120429872	0.3333571855138400	0.2116300064078296	T	T	T
0.6111699940000008	0.3888700010000008	0.00193000000000015	F	F	F
0.5556799769999969	0.4444999990000014	0.1067600029999980	F	F	F
0.4972461755235046	0.3314048916456779	0.2117274832222042	T	T	T
0.7777299879999973	0.3888300059999992	0.0018099999999990	F	F	F
0.7223399880000017	0.4443100089999987	0.1068800019999969	F	F	F
0.6667502870110195	0.3327124603878421	0.2075429138570614	T	T	T
0.9442700150000007	0.3886499999999984	0.00153000000000025	F	F	F
0.8888400200000035	0.4441399869999998	0.10661000000000034	F	F	F
0.8335125061302016	0.3346355264670840	0.2119392800575363	T	T	T
0.1107399990000033	0.5554000139999999	0.0015399999999985	F	F	F
0.0553000009999991	0.6110699769999997	0.1064700040000019	F	F	F
0.9977944483454398	0.4998435546998707	0.2116290757905335	T	T	T
0.2775200009999992	0.5554400090000016	0.00151000000000032	F	F	F
0.2220100019999975	0.6111699940000008	0.1063100029999973	F	F	F
0.1652029140759449	0.4996530186226031	0.2115994366560635	T	T	T
0.4443199930000006	0.5553799870000020	0.00159000000000002	F	F	F
0.3887799979999969	0.6112400290000011	0.1062999959999971	F	F	F
0.3311838761932667	0.4997096318513652	0.2114656441415668	T	T	T
0.6111099720000013	0.5553699729999977	0.00175000000000013	F	F	F
0.5554999710000033	0.6111999749999981	0.1063600029999989	F	F	F
0.4961170935368762	0.4991517587489485	0.2106483939400273	T	T	T
0.7778999809999974	0.5554400090000016	0.00195000000000008	F	F	F
0.7222300170000011	0.6110600230000003	0.1066500020000021	F	F	F
0.6612856605661095	0.4968612422182176	0.2124542287479075	T	T	T
0.9445199970000004	0.5554299949999972	0.00198999999999993	F	F	F
0.8888599870000036	0.6110200290000023	0.1069499999999977	F	F	F
0.8251064286921844	0.4983420887504501	0.2251323155675392	T	T	T
0.1105400029999970	0.7220600249999976	0.0015399999999985	F	F	F
0.0551999990000027	0.7777100209999972	0.1065599989999981	F	F	F
0.0017450642472715	0.6661738502874549	0.2107459782867729	T	T	T
0.2772899870000032	0.7220399979999996	0.0013099999999966	F	F	F
0.2219100000000012	0.7778099780000005	0.10627000000000021	F	F	F
0.1658042968326681	0.6652084509326727	0.2114002649417386	T	T	T
0.4440500139999983	0.7219600080000035	0.00122000000000036	F	F	F

0.3886399869999977	0.7778999809999974	0.1059899999999985	F	F	F
0.3316865449910549	0.6657883765615480	0.2112635566267669	T	T	T
0.6109200120000011	0.7219100000000012	0.0012899999999973	F	F	F
0.5553399920000004	0.7779099939999981	0.1059399990000003	F	F	F
0.4966649040780159	0.6665507297209731	0.2101730140201536	T	T	T
0.7777699829999989	0.7219200130000019	0.0015900000000002	F	F	F
0.7220399979999996	0.7778499719999985	0.1060900020000020	F	F	F
0.6628468205714216	0.6675184181103010	0.2185110246026900	T	T	T
0.9445099830000032	0.7220100159999987	0.0019899999999993	F	F	F
0.8887400030000023	0.7777600289999995	0.1066000009999968	F	F	F
0.8398683118843666	0.6727771851211668	0.2177747329656439	T	T	T
0.1104200039999981	0.8887100219999979	0.0016499999999979	F	F	F
0.0551300010000020	0.9443600179999976	0.1066899969999966	F	F	F
0.0031328095759625	0.8364432979252102	0.2098472771762604	T	T	T
0.2770999970000005	0.8887100219999979	0.0012699999999981	F	F	F
0.2218199969999972	0.9444400069999972	0.1063499970000024	F	F	F
0.1648278783375001	0.8302639919990401	0.2104849334494770	T	T	T
0.4438599940000003	0.8886200190000011	0.0009399999999999	F	F	F
0.3885099889999992	0.9445499779999977	0.1058700009999995	F	F	F
0.3324103881779690	0.8309642313264840	0.2103722401153149	T	T	T
0.6106699710000001	0.8884599800000004	0.0008100000000013	F	F	F
0.5552300209999999	0.9445899720000028	0.1055300009999982	F	F	F
0.4978587864033249	0.8317816713242826	0.2102139303606072	T	T	T
0.7774900200000019	0.8884199860000024	0.0009500000000031	F	F	F
0.7219899890000008	0.9445999860000001	0.1055099960000021	F	F	F
0.6651369742426291	0.8327505410443727	0.2090237570564415	T	T	T
0.9442700150000007	0.8884599800000004	0.0013500000000022	F	F	F
0.8886600140000027	0.9445499779999977	0.1058399980000004	F	F	F
0.8342886938487297	0.8353453060215009	0.2110967960553777	T	T	T
0.4239400029999985	0.0937699970000025	0.3320800070000018	F	F	F
0.6377458721304977	0.2986223194573705	0.3344143291160526	T	T	T
0.6439099910000010	0.0897099969999999	0.3303399979999995	F	F	F
0.4913099999999986	0.2268400040000031	0.3748100099999974	T	T	T
0.7083299760000017	0.2228900049999964	0.3731800019999980	T	T	T
0.5011900069999982	0.0272999999999968	0.3616600040000009	F	F	F
0.2867699860000030	0.0094399999999979	0.3104499880000020	F	F	F
0.6987400049999977	0.0066199999999981	0.3181200029999971	F	F	F
0.7542356192079254	0.4384877138978046	0.3774977479693392	T	T	T
0.7160850741426096	0.7049186067871888	0.3210917020261862	T	T	T
0.6347491621888056	0.5997762057416721	0.3201370921333930	T	T	T
0.6581857674981473	0.5171061448779037	0.3137311407911061	T	T	T
0.7655609640877969	0.5408272054488769	0.3030024098748066	T	T	T
0.8465735634649936	0.6455959538273175	0.3199138229870948	T	T	T
0.8222245060559614	0.7268107231001305	0.3218019595743313	T	T	T

0.7002448091776462	0.7641007024031092	0.3410872547647659	T	T	T
0.5586547185287267	0.5800607516956138	0.3404586184856391	T	T	T
0.6027940015054527	0.4456587014561228	0.3407002863571530	T	T	T
0.8817980609314072	0.8032247101601818	0.3396470530825204	T	T	T
0.8200041909274960	0.4389895695672162	0.3785875685403219	T	T	T
0.9216636224540007	0.6600330403009916	0.3387463594014342	T	T	T

phenyl\_hy\_mo3o5\_is

1.0000000000000000

14.9507999419999997 0.0000000000000000 0.0000000000000000

-7.4753999709999999 12.9477725567000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.0690994262999993

Ni Mo O C H

108 3 6 6 7

Selective dynamics

Direct

0.1111000029999971	0.0555500019999968	0.0018000000000029	F	F	F
0.0555500019999968	0.1111100019999967	0.1066899969999966	F	F	F
0.0008356310970505	0.0013213373404612	0.2111428263663119	T	T	T
0.2777900099999968	0.0555699989999994	0.0017899999999997	F	F	F
0.2222100050000009	0.1111000029999971	0.1066799979999971	F	F	F
0.1658952557917518	0.0007930489880546	0.2124143102327718	T	T	T
0.4444499909999990	0.0555500019999968	0.0018000000000029	F	F	F
0.3889000120000006	0.1111100019999967	0.1066799979999971	F	F	F
0.3299424920173199	0.9968754637171525	0.2148680179580269	T	T	T
0.6111000180000019	0.0555500019999968	0.0018000000000029	F	F	F
0.5555499789999985	0.1111100019999967	0.1067000030000003	F	F	F
0.4996972586459987	0.9997085002087449	0.2124014750298328	T	T	T
0.7777900099999968	0.0555699989999994	0.0017899999999997	F	F	F
0.7222099900000032	0.1111000029999971	0.1066799979999971	F	F	F
0.6682888715495684	0.9983704170288943	0.2178634107422334	T	T	T
0.9444500210000015	0.0555500019999968	0.0018000000000029	F	F	F
0.8888900279999987	0.1111000029999971	0.1066799979999971	F	F	F
0.8355168635398981	0.0001186381850968	0.2107755232078274	T	T	T
0.1111199999999997	0.2222400010000030	0.0018099999999990	F	F	F
0.0555599999999998	0.2777799959999996	0.1067200009999993	F	F	F
0.0004198134469879	0.1672122010357099	0.2115399499397915	T	T	T
0.2777900099999968	0.2222200040000004	0.0017899999999997	F	F	F
0.2222200040000004	0.2777799959999996	0.1067200009999993	F	F	F
0.1663607131879495	0.1675169104856417	0.2114855536897372	T	T	T
0.4444299939999965	0.2222100050000009	0.0017899999999997	F	F	F
0.3889000120000006	0.2777900099999968	0.1066799979999971	F	F	F
0.3338545167683536	0.1695011309637862	0.2109953593800955	T	T	T
0.6111199859999985	0.2222400010000030	0.0018099999999990	F	F	F
0.5555599930000028	0.2777799959999996	0.1067200009999993	F	F	F
0.5023790246870383	0.1690197835856476	0.2160880213922789	T	T	T
0.7777799959999996	0.2222100050000009	0.0017899999999997	F	F	F
0.7222200040000004	0.2777799959999996	0.1067200009999993	F	F	F
0.6669207883050645	0.1696964954643735	0.2137287097423538	T	T	T
0.9444299940000036	0.2222100050000009	0.0017899999999997	F	F	F
0.8888999819999981	0.2777900099999968	0.1066799979999971	F	F	F

0.8351316912001229	0.1692279608179189	0.2110508249035486	T	T	T
0.1111199999999997	0.3888800140000015	0.0018099999999990	F	F	F
0.0555599999999998	0.4444499909999990	0.1066899969999966	F	F	F
0.0001908833699532	0.3336218365296861	0.2114182523574634	T	T	T
0.2777599989999970	0.3888800140000015	0.0018099999999990	F	F	F
0.2222200040000004	0.4444400069999972	0.1067200009999993	F	F	F
0.1662297498692697	0.3334341800558397	0.2117755181160851	T	T	T
0.4444499909999990	0.3889000120000006	0.0018000000000029	F	F	F
0.3888899980000033	0.4444499909999990	0.1066899969999966	F	F	F
0.3323166716376877	0.3332951408514698	0.2115991732032811	T	T	T
0.6111199859999985	0.3888800140000015	0.0018099999999990	F	F	F
0.5555599930000028	0.4444499909999990	0.1066899969999966	F	F	F
0.4996102911580551	0.3339282069818685	0.2122290701845667	T	T	T
0.7777600289999995	0.3888800140000015	0.0018099999999990	F	F	F
0.7222200040000004	0.4444400069999972	0.1067200009999993	F	F	F
0.6682153289974564	0.3362491462936313	0.2102314737745914	T	T	T
0.9444500210000015	0.3889000120000006	0.0018000000000029	F	F	F
0.8888900279999987	0.4444499909999990	0.1066899969999966	F	F	F
0.8337146007919158	0.3361232405373830	0.2131596781316728	T	T	T
0.1111000029999971	0.5555499789999985	0.0018000000000029	F	F	F
0.0555500019999968	0.6111099720000013	0.1066899969999966	F	F	F
-0.0000174885216952	0.4998691560910774	0.2131121420608354	T	T	T
0.2777900099999968	0.5555700059999964	0.0017899999999997	F	F	F
0.2222100050000009	0.6111000180000019	0.1066799979999971	F	F	F
0.1661068655306065	0.4996062536018571	0.2116146138470653	T	T	T
0.4444499909999990	0.5555499789999985	0.0018000000000029	F	F	F
0.3888899980000033	0.6111099720000013	0.1066799979999971	F	F	F
0.3314831323449541	0.4994003648352225	0.2116889574344331	T	T	T
0.6111000180000019	0.5555499789999985	0.0018000000000029	F	F	F
0.5555499789999985	0.6111099720000013	0.1066899969999966	F	F	F
0.4961347252826339	0.4986159623671677	0.2106386933642724	T	T	T
0.7777900099999968	0.5555700059999964	0.0017899999999997	F	F	F
0.7222099900000032	0.6111000180000019	0.1066799979999971	F	F	F
0.6640927450244550	0.5012250121689114	0.2150109595630384	T	T	T
0.9444500210000015	0.5555499789999985	0.0018000000000029	F	F	F
0.8888900279999987	0.6111099720000013	0.1066799979999971	F	F	F
0.8318126755858654	0.5057459699928569	0.2337929396837031	T	T	T
0.1111199999999997	0.7222399710000005	0.0018099999999990	F	F	F
0.0555599999999998	0.7777799959999996	0.1067200009999993	F	F	F
0.0049539191476464	0.6668227575985214	0.2107769069006499	T	T	T
0.2777900099999968	0.7222099900000032	0.0017899999999997	F	F	F
0.2222200040000004	0.7777799959999996	0.1067200009999993	F	F	F
0.1678383410311393	0.6659993464720386	0.2116225421427068	T	T	T
0.4444299939999965	0.7222200040000004	0.0017899999999997	F	F	F



0.3889000120000006	0.7777900099999968	0.1066799979999971	F	F	F
0.3324159028924847	0.6658165483114884	0.2116972494283558	T	T	T
0.6111199859999985	0.7222399710000005	0.0018099999999990	F	F	F
0.5555599930000028	0.7777799959999996	0.1067200009999993	F	F	F
0.4964440001094293	0.6659217519465440	0.2108839865542797	T	T	T
0.7777799959999996	0.7222200040000004	0.0017899999999997	F	F	F
0.7222200040000004	0.7777799959999996	0.1067200009999993	F	F	F
0.6608830641070390	0.6673404985177215	0.2182852820479241	T	T	T
0.9444299940000036	0.7222099900000032	0.0017899999999997	F	F	F
0.8888999819999981	0.7777900099999968	0.1066799979999971	F	F	F
0.8396002768648322	0.6701483013539641	0.2074332947123155	T	T	T
0.1111199999999997	0.8888800140000015	0.0018099999999990	F	F	F
0.0555500019999968	0.9444400069999972	0.1067000030000003	F	F	F
0.0035097366795373	0.8361151974949597	0.2103744216352139	T	T	T
0.2777599989999970	0.8888800140000015	0.0018099999999990	F	F	F
0.2222200040000004	0.9444400069999972	0.1067200009999993	F	F	F
0.1664093783982665	0.8311669696342885	0.2105008831685398	T	T	T
0.4444499909999990	0.8888999819999981	0.0018000000000029	F	F	F
0.3888899980000033	0.9444500210000015	0.1066899969999966	F	F	F
0.3335237820094433	0.8315815001486795	0.2109923325086502	T	T	T
0.6111199859999985	0.8888800140000015	0.0018099999999990	F	F	F
0.5555499789999985	0.9444500210000015	0.1066899969999966	F	F	F
0.4983618789438416	0.8320109562566718	0.2109937496178535	T	T	T
0.7777600289999995	0.8888800140000015	0.0018099999999990	F	F	F
0.7222200040000004	0.9444299940000036	0.1067200009999993	F	F	F
0.6654678081667643	0.8332715786992638	0.2099627820744775	T	T	T
0.9444500210000015	0.8888999819999981	0.0018000000000029	F	F	F
0.8888900279999987	0.9444500210000015	0.1067000030000003	F	F	F
0.8344726136440009	0.8317497610880217	0.2191697069485359	T	T	T
0.4241600040000009	0.0939899979999979	0.3321500119999996	F	F	F
0.6340399979999987	0.2950499949999994	0.3346000020000020	T	T	T
0.6458399890000024	0.0929699989999975	0.3316799999999986	F	F	F
0.4902299940000034	0.2273299989999984	0.3746300039999966	T	T	T
0.7098100190000025	0.2269300070000000	0.3737800119999974	T	T	T
0.5026999709999984	0.0292700010000004	0.3626599910000010	F	F	F
0.2870300109999988	0.0092500000000015	0.3105199929999998	F	F	F
0.7002000210000006	0.0093900000000033	0.3194699880000016	F	F	F
0.7254765438199563	0.4087046495657133	0.3975094720699748	T	T	T
0.7289762369427731	0.7384930203794400	0.3211090599682831	T	T	T
0.6562839063617617	0.6296758620138294	0.3228072064153459	T	T	T
0.6903880719697174	0.5553036857428897	0.3148470183380675	T	T	T
0.7975998286737462	0.5907367364523585	0.2955885949779088	T	T	T
0.8721014504522326	0.6992886259110875	0.3104659224952252	T	T	T
0.8380974521957086	0.7740569552329234	0.3209688530070908	T	T	T

0.7036303811599122	0.7912094549256210	0.3400400189333284	T	T	T
0.5802812500771942	0.6034268818139260	0.3459910111051264	T	T	T
0.6468644403516886	0.4832497932959091	0.3440539151329395	T	T	T
0.9514936482058349	0.7219146322494193	0.3255834207514893	T	T	T
0.8903005385013363	0.8470725783713080	0.3470842996008651	T	T	T
0.7690415352913315	0.3892782207461465	0.4241774354919843	T	T	T
0.9247178574160796	0.5016946187958892	0.2738872331097182	T	T	T

phenyl\_hy\_mo3o5\_ts

1.0000000000000000

14.9507999419999997 0.0000000000000000 0.0000000000000000

-7.4753999709999999 12.9477725567000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.0690994262999993

Ni Mo O C H

108 3 6 6 7

Selective dynamics

Direct

0.1111000029999971	0.0555500019999968	0.0018000000000029	F	F	F
0.0555500019999968	0.1111100019999967	0.1066899969999966	F	F	F
0.0008954542817260	0.0017076289942547	0.2111334525895787	T	T	T
0.2777900099999968	0.0555699989999994	0.0017899999999997	F	F	F
0.2222100050000009	0.1111000029999971	0.1066799979999971	F	F	F
0.1657806527964250	0.0007584618353995	0.2124272800654217	T	T	T
0.4444499909999990	0.0555500019999968	0.0018000000000029	F	F	F
0.3889000120000006	0.1111100019999967	0.1066799979999971	F	F	F
0.3296950892110673	0.9967382437647746	0.2148495554003162	T	T	T
0.6111000180000019	0.0555500019999968	0.0018000000000029	F	F	F
0.5555499789999985	0.1111100019999967	0.1067000030000003	F	F	F
0.4994940875149272	0.9997909435884670	0.2124388356158381	T	T	T
0.7777900099999968	0.0555699989999994	0.0017899999999997	F	F	F
0.7222099900000032	0.1111000029999971	0.1066799979999971	F	F	F
0.6682172444154406	0.9985378061521450	0.2178383853430411	T	T	T
0.9444500210000015	0.0555500019999968	0.0018000000000029	F	F	F
0.8888900279999987	0.1111000029999971	0.1066799979999971	F	F	F
0.8354624467772371	0.0007196922015088	0.2107460148510608	T	T	T
0.1111199999999997	0.2222400010000030	0.0018099999999990	F	F	F
0.0555599999999998	0.2777799959999996	0.1067200009999993	F	F	F
0.0004072165646510	0.1675275432647112	0.2115615076832982	T	T	T
0.2777900099999968	0.2222200040000004	0.0017899999999997	F	F	F
0.2222200040000004	0.2777799959999996	0.1067200009999993	F	F	F
0.1663591745606443	0.1676119358147449	0.2114616147548300	T	T	T
0.4444299939999965	0.2222100050000009	0.0017899999999997	F	F	F
0.3889000120000006	0.2777900099999968	0.1066799979999971	F	F	F
0.3338865820221538	0.1695657225402397	0.2109815913049979	T	T	T
0.6111199859999985	0.2222400010000030	0.0018099999999990	F	F	F
0.5555599930000028	0.2777799959999996	0.1067200009999993	F	F	F
0.5023332702869980	0.1690372706064102	0.2160529762902305	T	T	T
0.7777799959999996	0.2222100050000009	0.0017899999999997	F	F	F
0.7222200040000004	0.2777799959999996	0.1067200009999993	F	F	F
0.6667234835671620	0.1693932888791212	0.2134182512222804	T	T	T
0.9444299940000036	0.2222100050000009	0.0017899999999997	F	F	F
0.8888999819999981	0.2777900099999968	0.1066799979999971	F	F	F

0.8351099851419500	0.1694743113239457	0.2111051380857643	T	T	T
0.1111199999999997	0.3888800140000015	0.0018099999999990	F	F	F
0.0555599999999998	0.4444499909999990	0.1066899969999966	F	F	F
-0.0001066170525367	0.3341245610746960	0.2115531536783253	T	T	T
0.2777599989999970	0.3888800140000015	0.0018099999999990	F	F	F
0.2222200040000004	0.4444400069999972	0.1067200009999993	F	F	F
0.1660638094386648	0.3334915498373243	0.2118370849857125	T	T	T
0.4444499909999990	0.3889000120000006	0.0018000000000029	F	F	F
0.3888899980000033	0.4444499909999990	0.1066899969999966	F	F	F
0.3322853412956029	0.3333911565497453	0.2115941417489312	T	T	T
0.6111199859999985	0.3888800140000015	0.0018099999999990	F	F	F
0.5555599930000028	0.4444499909999990	0.1066899969999966	F	F	F
0.4997590502490130	0.3339871770014542	0.2122769575472607	T	T	T
0.7777600289999995	0.3888800140000015	0.0018099999999990	F	F	F
0.7222200040000004	0.4444400069999972	0.1067200009999993	F	F	F
0.6685101328947420	0.3364188772263236	0.2108460890568562	T	T	T
0.9444500210000015	0.3889000120000006	0.0018000000000029	F	F	F
0.8888900279999987	0.4444499909999990	0.1066899969999966	F	F	F
0.8335165117872425	0.3362994273663222	0.2124866626035935	T	T	T
0.1111000029999971	0.5555499789999985	0.0018000000000029	F	F	F
0.0555500019999968	0.6111099720000013	0.1066899969999966	F	F	F
-0.0009568508812897	0.4999593121147728	0.2127934422779522	T	T	T
0.2777900099999968	0.5555700059999964	0.0017899999999997	F	F	F
0.2222100050000009	0.6111000180000019	0.1066799979999971	F	F	F
0.1657113470501204	0.4996196636197947	0.2117082247706193	T	T	T
0.4444499909999990	0.5555499789999985	0.0018000000000029	F	F	F
0.3888899980000033	0.6111099720000013	0.1066799979999971	F	F	F
0.3311929775869848	0.4993918728258150	0.2117257358148571	T	T	T
0.6111000180000019	0.5555499789999985	0.0018000000000029	F	F	F
0.5555499789999985	0.6111099720000013	0.1066899969999966	F	F	F
0.4959194612080006	0.4988221267541632	0.2107275486982603	T	T	T
0.7777900099999968	0.5555700059999964	0.0017899999999997	F	F	F
0.7222099900000032	0.6111000180000019	0.1066799979999971	F	F	F
0.6632807629364000	0.5011922535421972	0.2156907475743707	T	T	T
0.9444500210000015	0.5555499789999985	0.0018000000000029	F	F	F
0.8888900279999987	0.6111099720000013	0.1066799979999971	F	F	F
0.8330748483179437	0.5078299001887143	0.2326877638976092	T	T	T
0.1111199999999997	0.7222399710000005	0.0018099999999990	F	F	F
0.0555599999999998	0.7777799959999996	0.1067200009999993	F	F	F
0.0042813783092947	0.6663722344707510	0.2108730977593780	T	T	T
0.2777900099999968	0.7222099900000032	0.0017899999999997	F	F	F
0.2222200040000004	0.7777799959999996	0.1067200009999993	F	F	F
0.1671804968579837	0.6657417480771689	0.2117212016371817	T	T	T
0.4444299939999965	0.7222200040000004	0.0017899999999997	F	F	F

0.3889000120000006	0.7777900099999968	0.1066799979999971	F	F	F
0.3320411370380525	0.6658851643217031	0.2117089088719864	T	T	T
0.6111199859999985	0.7222399710000005	0.0018099999999990	F	F	F
0.5555599930000028	0.7777799959999996	0.1067200009999993	F	F	F
0.4959755211100053	0.6660611101153894	0.2107856729850998	T	T	T
0.7777799959999996	0.7222200040000004	0.0017899999999997	F	F	F
0.7222200040000004	0.7777799959999996	0.1067200009999993	F	F	F
0.6604556539005484	0.6677285647579139	0.2180437011622287	T	T	T
0.9444299940000036	0.7222099900000032	0.0017899999999997	F	F	F
0.8888999819999981	0.7777900099999968	0.1066799979999971	F	F	F
0.8385541969629228	0.6721707499668633	0.2070576571494340	T	T	T
0.1111199999999997	0.8888800140000015	0.0018099999999990	F	F	F
0.0555500019999968	0.9444400069999972	0.1067000030000003	F	F	F
0.0032610445580402	0.8362948365819710	0.2104203618996075	T	T	T
0.2777599989999970	0.8888800140000015	0.0018099999999990	F	F	F
0.2222200040000004	0.9444400069999972	0.1067200009999993	F	F	F
0.1659073223223045	0.8309001115782343	0.2104785199053795	T	T	T
0.4444499909999990	0.8888999819999981	0.0018000000000029	F	F	F
0.3888899980000033	0.9444500210000015	0.1066899969999966	F	F	F
0.3332174340226823	0.8315457668150145	0.2109659471106894	T	T	T
0.6111199859999985	0.8888800140000015	0.0018099999999990	F	F	F
0.5555499789999985	0.9444500210000015	0.1066899969999966	F	F	F
0.4981581426491678	0.8322032754169113	0.2109501431993256	T	T	T
0.7777600289999995	0.8888800140000015	0.0018099999999990	F	F	F
0.7222200040000004	0.9444299940000036	0.1067200009999993	F	F	F
0.6651751549591000	0.8336086881748119	0.2099346493958313	T	T	T
0.9444500210000015	0.8888999819999981	0.0018000000000029	F	F	F
0.8888900279999987	0.9444500210000015	0.1067000030000003	F	F	F
0.8343347611112626	0.8332736524415315	0.2183439643444103	T	T	T
0.4241600040000009	0.0939899979999979	0.3321500119999996	F	F	F
0.6364012139676272	0.3017415646133656	0.3378630611961230	T	T	T
0.6458399890000024	0.0929699989999975	0.3316799999999986	F	F	F
0.4902299940000034	0.2273299989999984	0.3746300039999966	T	T	T
0.7098100190000025	0.2269300070000000	0.3737800119999974	T	T	T
0.5026999709999984	0.0292700010000004	0.3626599910000010	F	F	F
0.2870300109999988	0.0092500000000015	0.3105199929999998	F	F	F
0.7002000210000006	0.0093900000000033	0.3194699880000016	F	F	F
0.7304871968245861	0.4119898589111485	0.4022803874261550	T	T	T
0.7213518727815356	0.7331908513796295	0.3203950111158702	T	T	T
0.6541160939054127	0.6233486036203156	0.3215692427924799	T	T	T
0.6943986178726236	0.5532661296685182	0.3150840261266529	T	T	T
0.8034735888313005	0.5955058715372876	0.2965940322906059	T	T	T
0.8722687778536973	0.7056589235942539	0.3097459716306614	T	T	T
0.8317966397732942	0.7753204181068957	0.3198877946089113	T	T	T

0.6914970940777229	0.7823355196332248	0.3392054783972096	T	T	T
0.5769198137406005	0.5927672841221822	0.3439969661460369	T	T	T
0.6561341389498753	0.4842884289901799	0.3478264449267603	T	T	T
0.9529995662731888	0.7338920157224335	0.3243598800614946	T	T	T
0.8803208380822972	0.8489756870060459	0.3465506127956242	T	T	T
0.7704750128986306	0.3886071977022238	0.4293821711712920	T	T	T
0.8955067654504461	0.5489197452775676	0.2985285985703108	T	T	T

phenol\_ddo\_mo3o7\_is

1.0000000000000000

14.9507999419999997 0.0000000000000000 0.0000000000000000

-7.4753999709999999 12.9477725567000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.0690994262999993

Ni Mo O C H  
108 3 8 6 6

Selective dynamics

Direct

0.1111000029999971	0.0555500019999968	0.0018000000000029	F	F	F
0.0555500019999968	0.1111100019999967	0.1066899969999966	F	F	F
0.0009755415813348	0.0006299489934784	0.2110547414881294	T	T	T
0.2777900099999968	0.0555699989999994	0.0017899999999997	F	F	F
0.2222100050000009	0.1111000029999971	0.1066799979999971	F	F	F
0.1649896636095607	0.9991463059077343	0.2165476948235323	T	T	T
0.4444499909999990	0.0555500019999968	0.0018000000000029	F	F	F
0.3889000120000006	0.1111100019999967	0.1066799979999971	F	F	F
0.3322911317603618	0.9954501564001231	0.2105966330865426	T	T	T
0.6111000180000019	0.0555500019999968	0.0018000000000029	F	F	F
0.5555499789999985	0.1111100019999967	0.1067000030000003	F	F	F
0.4992339184303495	0.9981723969733028	0.2203745003198889	T	T	T
0.7777900099999968	0.0555699989999994	0.0017899999999997	F	F	F
0.7222099900000032	0.1111000029999971	0.1066799979999971	F	F	F
0.6630358708076981	0.9971942574481302	0.2123071137847021	T	T	T
0.9444500210000015	0.0555500019999968	0.0018000000000029	F	F	F
0.8888900279999987	0.1111000029999971	0.1066799979999971	F	F	F
0.8357600099739980	0.0001238981025528	0.2151435095169240	T	T	T
0.1111199999999997	0.2222400010000030	0.0018099999999990	F	F	F
0.0555599999999998	0.2777799959999996	0.1067200009999993	F	F	F
0.0034503710315900	0.1690203268590317	0.2109740967758411	T	T	T
0.2777900099999968	0.2222200040000004	0.0017899999999997	F	F	F
0.2222200040000004	0.2777799959999996	0.1067200009999993	F	F	F
0.1659583290593916	0.1688908604575659	0.2110553412602972	T	T	T
0.4444299939999965	0.2222100050000009	0.0017899999999997	F	F	F
0.3889000120000006	0.2777900099999968	0.1066799979999971	F	F	F
0.3350521818086156	0.1705830666069620	0.2148856971169503	T	T	T
0.6111199859999985	0.2222400010000030	0.0018099999999990	F	F	F
0.5555599930000028	0.2777799959999996	0.1067200009999993	F	F	F
0.5026571791239312	0.1682201195701143	0.2101390962472049	T	T	T
0.7777799959999996	0.2222100050000009	0.0017899999999997	F	F	F
0.7222200040000004	0.2777799959999996	0.1067200009999993	F	F	F
0.6667005281575169	0.1689845962617972	0.2107877303976478	T	T	T
0.9444299940000036	0.2222100050000009	0.0017899999999997	F	F	F
0.8888999819999981	0.2777900099999968	0.1066799979999971	F	F	F



0.8358326008446867	0.1708174766482264	0.2143353406838095	T	T	T
0.1111199999999997	0.3888800140000015	0.0018099999999990	F	F	F
0.0555599999999998	0.4444499909999990	0.1066899969999966	F	F	F
0.0011903060626177	0.3343595745983339	0.2113500525759254	T	T	T
0.2777599989999970	0.3888800140000015	0.0018099999999990	F	F	F
0.2222200040000004	0.4444400069999972	0.1067200009999993	F	F	F
0.1679414760222250	0.3348460300027526	0.2117810570580421	T	T	T
0.4444499909999990	0.3889000120000006	0.0018000000000029	F	F	F
0.3888899980000033	0.4444499909999990	0.1066899969999966	F	F	F
0.3339774545827648	0.3344063379275359	0.2109969118347810	T	T	T
0.6111199859999985	0.3888800140000015	0.0018099999999990	F	F	F
0.5555599930000028	0.4444499909999990	0.1066899969999966	F	F	F
0.4990600298248915	0.3315053073333061	0.2089343149035405	T	T	T
0.7777600289999995	0.3888800140000015	0.0018099999999990	F	F	F
0.7222200040000004	0.4444400069999972	0.1067200009999993	F	F	F
0.6686513809403635	0.3320782938505286	0.2108087071976877	T	T	T
0.9444500210000015	0.3889000120000006	0.0018000000000029	F	F	F
0.8888900279999987	0.4444499909999990	0.1066899969999966	F	F	F
0.8346322515052943	0.3343763286142232	0.2123125691208264	T	T	T
0.1111000029999971	0.5555499789999985	0.0018000000000029	F	F	F
0.0555500019999968	0.6111099720000013	0.1066899969999966	F	F	F
0.0007319781729180	0.5000800876045745	0.2117431990810259	T	T	T
0.2777900099999968	0.5555700059999964	0.0017899999999997	F	F	F
0.2222100050000009	0.6111000180000019	0.1066799979999971	F	F	F
0.1667649484506362	0.4997408541237254	0.2117788522836321	T	T	T
0.4444499909999990	0.5555499789999985	0.0018000000000029	F	F	F
0.3888899980000033	0.6111099720000013	0.1066799979999971	F	F	F
0.3333400434750079	0.4998794379706351	0.2113022616710576	T	T	T
0.6111000180000019	0.5555499789999985	0.0018000000000029	F	F	F
0.5555499789999985	0.6111099720000013	0.1066899969999966	F	F	F
0.5025828363488807	0.5005541494583913	0.2181027226615043	T	T	T
0.7777900099999968	0.5555700059999964	0.0017899999999997	F	F	F
0.7222099900000032	0.6111000180000019	0.1066799979999971	F	F	F
0.6675747099471330	0.4939996896399249	0.2193213139641249	T	T	T
0.9444500210000015	0.5555499789999985	0.0018000000000029	F	F	F
0.8888900279999987	0.6111099720000013	0.1066799979999971	F	F	F
0.8353774836840310	0.4991452255093205	0.2111683041502312	T	T	T
0.1111199999999997	0.7222399710000005	0.0018099999999990	F	F	F
0.0555599999999998	0.7777799959999996	0.1067200009999993	F	F	F
-0.0001365309489648	0.6661300724742378	0.2111469371133327	T	T	T
0.2777900099999968	0.7222099900000032	0.0017899999999997	F	F	F
0.2222200040000004	0.7777799959999996	0.1067200009999993	F	F	F
0.1659840559307797	0.6652357184945524	0.2118533937297133	T	T	T
0.4444299939999965	0.7222200040000004	0.0017899999999997	F	F	F

0.3889000120000006	0.7777900099999968	0.1066799979999971	F	F	F
0.3320406162042546	0.6655946864921283	0.2115804183209275	T	T	T
0.6111199859999985	0.7222399710000005	0.0018099999999990	F	F	F
0.5555599930000028	0.7777799959999996	0.1067200009999993	F	F	F
0.4972350733388764	0.6664407461237186	0.2107251356378103	T	T	T
0.7777799959999996	0.7222200040000004	0.0017899999999997	F	F	F
0.7222200040000004	0.7777799959999996	0.1067200009999993	F	F	F
0.6660609343652886	0.6720408434461407	0.2172215001575312	T	T	T
0.9444299940000036	0.7222099900000032	0.0017899999999997	F	F	F
0.8888999819999981	0.7777900099999968	0.1066799979999971	F	F	F
0.8323774424768242	0.6667317242885828	0.2171346506796228	T	T	T
0.1111199999999997	0.8888800140000015	0.0018099999999990	F	F	F
0.0555500019999968	0.9444400069999972	0.1067000030000003	F	F	F
0.0003379992169069	0.8332531514057505	0.2108933068025292	T	T	T
0.2777599989999970	0.8888800140000015	0.0018099999999990	F	F	F
0.2222200040000004	0.9444400069999972	0.1067200009999993	F	F	F
0.1639796781906003	0.8291138264766292	0.2111895560309029	T	T	T
0.4444499909999990	0.8888999819999981	0.0018000000000029	F	F	F
0.3888899980000033	0.9444500210000015	0.1066899969999966	F	F	F
0.3311089145493655	0.8302619421536586	0.2116476255748151	T	T	T
0.6111199859999985	0.8888800140000015	0.0018099999999990	F	F	F
0.5555499789999985	0.9444500210000015	0.1066899969999966	F	F	F
0.4977964900932189	0.8306608969823207	0.2110502267753081	T	T	T
0.7777600289999995	0.8888800140000015	0.0018099999999990	F	F	F
0.7222200040000004	0.9444299940000036	0.1067200009999993	F	F	F
0.6650253793529575	0.8333500832734204	0.2091659998426043	T	T	T
0.9444500210000015	0.8888999819999981	0.0018000000000029	F	F	F
0.8888900279999987	0.9444500210000015	0.1067000030000003	F	F	F
0.8350307797358920	0.8357485515301872	0.2103013401999946	T	T	T
0.3862099950000015	0.0252100009999978	0.3365699949999978	F	F	F
0.6254069397283126	0.2425180816562270	0.3343528402539597	T	T	T
0.6537299749999974	0.0397999990000031	0.3406400080000012	F	F	F
0.4810299869999994	0.1689800019999979	0.3683600130000002	T	T	T
0.6999099849999979	0.1711699960000033	0.3778100010000003	T	T	T
0.5097600220000018	0.9990599750000015	0.3261699970000009	F	F	F
0.2878499930000018	0.0602600019999997	0.2814300060000008	F	F	F
0.7732499840000031	0.0595900009999966	0.2837100030000030	F	F	F
0.6486700179999971	0.9545300010000020	0.4026600119999983	F	F	F
0.3127700089999976	0.9412000180000035	0.4012300070000023	F	F	F
0.5800973589257655	0.3783850204735520	0.3551837996923730	T	T	T
0.7226755682824320	0.6967091304416470	0.3197324805918347	T	T	T
0.6120897959809520	0.6369364686320734	0.3200349046004984	T	T	T
0.5579826929821535	0.5246356757084990	0.3213017759388944	T	T	T
0.6213883922387632	0.4767508542509073	0.3257620390201315	T	T	T

0.7313189163279089	0.5352449976427611	0.3218588711890806	T	T	T
0.7847951703923255	0.6471243747717534	0.3197212552625521	T	T	T
0.7594486016174836	0.7777137272971514	0.3360516182033583	T	T	T
0.5686955162814578	0.6744656500029356	0.3364371199438095	T	T	T
0.4824521469352532	0.4849866510329930	0.3473334842957149	T	T	T
0.8616895321373689	0.6884718331250465	0.3435886030988368	T	T	T
0.5042908673161431	0.3376096605081316	0.3499682762270730	T	T	T
0.7743267051395465	0.4979566911055228	0.3394305102732255	T	T	T

phenol\_ddo\_mo3o7\_ts

1.0000000000000000

14.9507999419999997 0.0000000000000000 0.0000000000000000

-7.4753999709999999 12.9477725567000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.0690994262999993

Ni Mo O C H

108 3 8 6 6

Selective dynamics

Direct

0.1111000029999971	0.0555500019999968	0.0018000000000029	F	F	F
0.0555500019999968	0.1111100019999967	0.1066899969999966	F	F	F
0.0012710355498478	0.0009031497388312	0.2110514534617588	T	T	T
0.2777900099999968	0.0555699989999994	0.0017899999999997	F	F	F
0.2222100050000009	0.1111000029999971	0.1066799979999971	F	F	F
0.1657812153845374	1.0000301158102356	0.2166513825017392	T	T	T
0.4444499909999990	0.0555500019999968	0.0018000000000029	F	F	F
0.3889000120000006	0.1111100019999967	0.1066799979999971	F	F	F
0.3325762018398607	0.9966741193722615	0.2098884324002843	T	T	T
0.6111000180000019	0.0555500019999968	0.0018000000000029	F	F	F
0.5555499789999985	0.1111100019999967	0.1067000030000003	F	F	F
0.4993486133225948	0.9990071533244650	0.2203867522194597	T	T	T
0.7777900099999968	0.0555699989999994	0.0017899999999997	F	F	F
0.7222099900000032	0.1111000029999971	0.1066799979999971	F	F	F
0.6630434512123405	0.9979188587002454	0.2121495065918074	T	T	T
0.9444500210000015	0.0555500019999968	0.0018000000000029	F	F	F
0.8888900279999987	0.1111000029999971	0.1066799979999971	F	F	F
0.8358129017207302	0.0004370521558302	0.2152164127680679	T	T	T
0.1111199999999997	0.2222400010000030	0.0018099999999990	F	F	F
0.0555599999999998	0.2777799959999996	0.1067200009999993	F	F	F
0.0035221124212471	0.1689907000813488	0.2110161364167432	T	T	T
0.2777900099999968	0.2222200040000004	0.0017899999999997	F	F	F
0.2222200040000004	0.2777799959999996	0.1067200009999993	F	F	F
0.1665085473059553	0.1691509887787143	0.2110526907993028	T	T	T
0.4444299939999965	0.2222100050000009	0.0017899999999997	F	F	F
0.3889000120000006	0.2777900099999968	0.1066799979999971	F	F	F
0.3373410246532602	0.1722860041541659	0.2150981029006392	T	T	T
0.6111199859999985	0.2222400010000030	0.0018099999999990	F	F	F
0.5555599930000028	0.2777799959999996	0.1067200009999993	F	F	F
0.5037048579401932	0.1699334266105509	0.2107785773987991	T	T	T
0.7777799959999996	0.2222100050000009	0.0017899999999997	F	F	F
0.7222200040000004	0.2777799959999996	0.1067200009999993	F	F	F
0.6670203024779091	0.1694519519445865	0.2107525557833551	T	T	T
0.9444299940000036	0.2222100050000009	0.0017899999999997	F	F	F
0.8888999819999981	0.2777900099999968	0.1066799979999971	F	F	F

0.8359502437300519	0.1709718299462045	0.2143223749989238	T	T	T
0.1111199999999997	0.3888800140000015	0.0018099999999990	F	F	F
0.0555599999999998	0.4444499909999990	0.1066899969999966	F	F	F
0.0013098896651269	0.3344027567482275	0.2113689251962510	T	T	T
0.2777599989999970	0.3888800140000015	0.0018099999999990	F	F	F
0.2222200040000004	0.4444400069999972	0.1067200009999993	F	F	F
0.1678223083057565	0.3348281720021559	0.2118518373194743	T	T	T
0.4444499909999990	0.3889000120000006	0.0018000000000029	F	F	F
0.3888899980000033	0.4444499909999990	0.1066899969999966	F	F	F
0.3343582136129899	0.3346199571820911	0.2107539796537918	T	T	T
0.6111199859999985	0.3888800140000015	0.0018099999999990	F	F	F
0.5555599930000028	0.4444499909999990	0.1066899969999966	F	F	F
0.5057240825062509	0.3387295382716300	0.2194378060698442	T	T	T
0.7777600289999995	0.3888800140000015	0.0018099999999990	F	F	F
0.7222200040000004	0.4444400069999972	0.1067200009999993	F	F	F
0.6698004763650683	0.3324716242682851	0.2096424636269958	T	T	T
0.9444500210000015	0.3889000120000006	0.0018000000000029	F	F	F
0.8888900279999987	0.4444499909999990	0.1066899969999966	F	F	F
0.8351312026228284	0.3344772626670189	0.2123183712075715	T	T	T
0.1111000029999971	0.5555499789999985	0.0018000000000029	F	F	F
0.0555500019999968	0.6111099720000013	0.1066899969999966	F	F	F
0.0010671151828504	0.5002892796966097	0.2117685097850877	T	T	T
0.2777900099999968	0.5555700059999964	0.0017899999999997	F	F	F
0.2222100050000009	0.6111000180000019	0.1066799979999971	F	F	F
0.1666405446652101	0.4998488828988793	0.2118389257124787	T	T	T
0.4444499909999990	0.5555499789999985	0.0018000000000029	F	F	F
0.3888899980000033	0.6111099720000013	0.1066799979999971	F	F	F
0.3328783588085225	0.5000255722230192	0.2113109825395722	T	T	T
0.6111000180000019	0.5555499789999985	0.0018000000000029	F	F	F
0.5555499789999985	0.6111099720000013	0.1066899969999966	F	F	F
0.5012590346522343	0.5026644631522812	0.2161792383917651	T	T	T
0.7777900099999968	0.5555700059999964	0.0017899999999997	F	F	F
0.7222099900000032	0.6111000180000019	0.1066799979999971	F	F	F
0.6701744882037615	0.4984793034748461	0.2111925751245189	T	T	T
0.9444500210000015	0.5555499789999985	0.0018000000000029	F	F	F
0.8888900279999987	0.6111099720000013	0.1066799979999971	F	F	F
0.8366493985225533	0.4996823079422504	0.2116910986140842	T	T	T
0.1111199999999997	0.7222399710000005	0.0018099999999990	F	F	F
0.0555599999999998	0.7777799959999996	0.1067200009999993	F	F	F
1.0004331764914201	0.6666802972470069	0.2112318690721076	T	T	T
0.2777900099999968	0.7222099900000032	0.0017899999999997	F	F	F
0.2222200040000004	0.7777799959999996	0.1067200009999993	F	F	F
0.1660859197581932	0.6654935690575036	0.2118581176452776	T	T	T
0.4444299939999965	0.7222200040000004	0.0017899999999997	F	F	F

0.3889000120000006	0.7777900099999968	0.1066799979999971	F	F	F
0.3317628961571386	0.6659015225745456	0.2115935923503907	T	T	T
0.6111199859999985	0.7222399710000005	0.0018099999999990	F	F	F
0.5555599930000028	0.7777799959999996	0.1067200009999993	F	F	F
0.4969656777033593	0.6674418139946318	0.2108809040309839	T	T	T
0.7777799959999996	0.7222200040000004	0.0017899999999997	F	F	F
0.7222200040000004	0.7777799959999996	0.1067200009999993	F	F	F
0.6657684046502381	0.6737618851486028	0.2183289464856547	T	T	T
0.9444299940000036	0.7222099900000032	0.0017899999999997	F	F	F
0.8888999819999981	0.7777900099999968	0.1066799979999971	F	F	F
0.8331618191261723	0.6680391807254850	0.2178839792483852	T	T	T
0.1111199999999997	0.8888800140000015	0.0018099999999990	F	F	F
0.0555500019999968	0.9444400069999972	0.1067000030000003	F	F	F
0.0007473035338437	0.8337130790871760	0.2110079041294698	T	T	T
0.2777599989999970	0.8888800140000015	0.0018099999999990	F	F	F
0.2222200040000004	0.9444400069999972	0.1067200009999993	F	F	F
0.1644077162087260	0.8296396959127758	0.2111965272270039	T	T	T
0.4444499909999990	0.8888999819999981	0.0018000000000029	F	F	F
0.3888899980000033	0.9444500210000015	0.1066899969999966	F	F	F
0.3312947053435132	0.8308924587179847	0.2116028107129740	T	T	T
0.6111199859999985	0.8888800140000015	0.0018099999999990	F	F	F
0.5555499789999985	0.9444500210000015	0.1066899969999966	F	F	F
0.4977957398881503	0.8313843977967228	0.2110687609667817	T	T	T
0.7777600289999995	0.8888800140000015	0.0018099999999990	F	F	F
0.7222200040000004	0.9444299940000036	0.1067200009999993	F	F	F
0.6651361964397540	0.8340346966648677	0.2093867323533392	T	T	T
0.9444500210000015	0.8888999819999981	0.0018000000000029	F	F	F
0.8888900279999987	0.9444500210000015	0.1067000030000003	F	F	F
0.8352566261193927	0.8361552377436294	0.2103809054806380	T	T	T
0.3862099950000015	0.0252100009999978	0.3365699949999978	F	F	F
0.6214186772077758	0.2454900915795784	0.3333530250891422	T	T	T
0.6537299749999974	0.0397999990000031	0.3406400080000012	F	F	F
0.4743475409359825	0.1640007775543754	0.3689002260259688	T	T	T
0.6935720568385616	0.1700200987436217	0.3759910966236942	T	T	T
0.5097600220000018	0.9990599750000015	0.3261699970000009	F	F	F
0.2878499930000018	0.0602600019999997	0.2814300060000008	F	F	F
0.7732499840000031	0.0595900009999966	0.2837100030000030	F	F	F
0.6486700179999971	0.9545300010000020	0.4026600119999983	F	F	F
0.3127700089999976	0.9412000180000035	0.4012300070000023	F	F	F
0.6074360783972651	0.3647272417943777	0.3781140373661456	T	T	T
0.7193745619627344	0.6954765140026382	0.3219280175942323	T	T	T
0.6090912608887404	0.6343105350811421	0.3227339142306259	T	T	T
0.5552476677531214	0.5221575557263278	0.3174732915663728	T	T	T
0.6189162009456334	0.4760775617348658	0.3035617263568666	T	T	T

0.7310821615658616	0.5365941436599755	0.3110128305650428	T	T	T
0.7826049505698051	0.6472831987625699	0.3204275727146410	T	T	T
0.7551681248567114	0.7758797308630458	0.3392378663992065	T	T	T
0.5652136578726326	0.6707531045873339	0.3404357828010792	T	T	T
0.4798230046231425	0.4781379716277006	0.3429930700972053	T	T	T
0.8573072316946649	0.6857098406541112	0.3473709350044972	T	T	T
0.5363100785952383	0.3294166922328603	0.3960030140753442	T	T	T
0.7712460839147192	0.4968482563071906	0.3297294952341019	T	T	T

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-7.4753999709999999 12.9477725567000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.0690994262999993

Ni Mo O C H

108 3 8 6 7

Selective dynamics

Direct

0.1111000029999971	0.0555500019999968	0.0018000000000029	F	F	F
0.0555500019999968	0.1111100019999967	0.1066899969999966	F	F	F
0.0011743399730138	0.0009175895463246	0.2110605930940877	T	T	T
0.2777900099999968	0.0555699989999994	0.0017899999999997	F	F	F
0.2222100050000009	0.1111000029999971	0.1066799979999971	F	F	F
0.1659467182148672	0.0005484048753224	0.2162812272427672	T	T	T
0.4444499909999990	0.0555500019999968	0.0018000000000029	F	F	F
0.3889000120000006	0.1111100019999967	0.1066799979999971	F	F	F
0.3329485822321000	0.9970627963174514	0.2106358405424948	T	T	T
0.6111000180000019	0.0555500019999968	0.0018000000000029	F	F	F
0.5555499789999985	0.1111100019999967	0.1067000030000003	F	F	F
0.4997915443030339	0.9994949800564584	0.2202505910175424	T	T	T
0.7777900099999968	0.0555699989999994	0.0017899999999997	F	F	F
0.7222099900000032	0.1111000029999971	0.1066799979999971	F	F	F
0.6632335366644725	0.9980895435006291	0.2120175417710727	T	T	T
0.9444500210000015	0.0555500019999968	0.0018000000000029	F	F	F
0.8888900279999987	0.1111000029999971	0.1066799979999971	F	F	F
0.8357049621139671	0.0002642020928758	0.2152376864899686	T	T	T
0.1111199999999997	0.2222400010000030	0.0018099999999990	F	F	F
0.0555599999999998	0.2777799959999996	0.1067200009999993	F	F	F
0.0033370898305532	0.1692168617475633	0.2110037700976408	T	T	T
0.2777900099999968	0.2222200040000004	0.0017899999999997	F	F	F
0.2222200040000004	0.2777799959999996	0.1067200009999993	F	F	F
0.1658007251115100	0.1690177482779202	0.2108548964061236	T	T	T
0.4444299939999965	0.2222100050000009	0.0017899999999997	F	F	F
0.3889000120000006	0.2777900099999968	0.1066799979999971	F	F	F
0.3393489471999808	0.1745704887741583	0.2171997256231550	T	T	T
0.6111199859999985	0.2222400010000030	0.0018099999999990	F	F	F
0.5555599930000028	0.2777799959999996	0.1067200009999993	F	F	F
0.5041425007409444	0.1700704060095092	0.2104366746343982	T	T	T
0.7777799959999996	0.2222100050000009	0.0017899999999997	F	F	F
0.7222200040000004	0.2777799959999996	0.1067200009999993	F	F	F
0.6669971745310004	0.1701383676537204	0.2119350821543198	T	T	T
0.9444299940000036	0.2222100050000009	0.0017899999999997	F	F	F
0.8888999819999981	0.2777900099999968	0.1066799979999971	F	F	F



0.8358345774334425	0.1710390282086551	0.2143251591033805	T	T	T
0.1111199999999997	0.3888800140000015	0.0018099999999990	F	F	F
0.0555599999999998	0.4444499909999990	0.1066899969999966	F	F	F
0.0013388863884756	0.3346552321930460	0.2113231002108576	T	T	T
0.2777599989999970	0.3888800140000015	0.0018099999999990	F	F	F
0.2222200040000004	0.4444400069999972	0.1067200009999993	F	F	F
0.1677668777602008	0.3351642816629142	0.2117189923792280	T	T	T
0.4444499909999990	0.3889000120000006	0.0018000000000029	F	F	F
0.3888899980000033	0.4444499909999990	0.1066899969999966	F	F	F
0.3343963678436299	0.3357091365882965	0.2118006651026897	T	T	T
0.6111199859999985	0.3888800140000015	0.0018099999999990	F	F	F
0.5555599930000028	0.4444499909999990	0.1066899969999966	F	F	F
0.5119690552944616	0.3423052471721843	0.2347056510679300	T	T	T
0.7777600289999995	0.3888800140000015	0.0018099999999990	F	F	F
0.7222200040000004	0.4444400069999972	0.1067200009999993	F	F	F
0.6693207964427770	0.3319884196021547	0.2131586804027625	T	T	T
0.9444500210000015	0.3889000120000006	0.0018000000000029	F	F	F
0.8888900279999987	0.4444499909999990	0.1066899969999966	F	F	F
0.8353530317033269	0.3348539520062964	0.2121426229776913	T	T	T
0.1111000029999971	0.5555499789999985	0.0018000000000029	F	F	F
0.0555500019999968	0.6111099720000013	0.1066899969999966	F	F	F
0.0008790447107173	0.5006173025169007	0.2117175604609897	T	T	T
0.2777900099999968	0.5555700059999964	0.0017899999999997	F	F	F
0.2222100050000009	0.6111000180000019	0.1066799979999971	F	F	F
0.1664349816335461	0.5002341947957840	0.2118088353979548	T	T	T
0.4444499909999990	0.5555499789999985	0.0018000000000029	F	F	F
0.3888899980000033	0.6111099720000013	0.1066799979999971	F	F	F
0.3322757504851381	0.5005283498021137	0.2110096211677610	T	T	T
0.6111000180000019	0.5555499789999985	0.0018000000000029	F	F	F
0.5555499789999985	0.6111099720000013	0.1066899969999966	F	F	F
0.5004851176337607	0.5035832545786596	0.2132449645078544	T	T	T
0.7777900099999968	0.5555700059999964	0.0017899999999997	F	F	F
0.7222099900000032	0.6111000180000019	0.1066799979999971	F	F	F
0.6712230668494091	0.5015687324641254	0.2078430829940318	T	T	T
0.9444500210000015	0.5555499789999985	0.0018000000000029	F	F	F
0.8888900279999987	0.6111099720000013	0.1066799979999971	F	F	F
0.8361914198639238	0.4998611313783220	0.2108270711864826	T	T	T
0.1111199999999997	0.7222399710000005	0.0018099999999990	F	F	F
0.0555599999999998	0.7777799959999996	0.1067200009999993	F	F	F
0.9997066144197231	0.6668402502586800	0.2113685769206660	T	T	T
0.2777900099999968	0.7222099900000032	0.0017899999999997	F	F	F
0.2222200040000004	0.7777799959999996	0.1067200009999993	F	F	F
0.1659328414452469	0.6658420809790493	0.2118104740875847	T	T	T
0.4444299939999965	0.7222200040000004	0.0017899999999997	F	F	F

0.3889000120000006	0.7777900099999968	0.1066799979999971	F	F	F
0.3317842583227685	0.6663712175688887	0.2115614685765069	T	T	T
0.6111199859999985	0.7222399710000005	0.0018099999999990	F	F	F
0.5555599930000028	0.7777799959999996	0.1067200009999993	F	F	F
0.4972395555980660	0.6679713788631665	0.2111019192515036	T	T	T
0.7777799959999996	0.7222200040000004	0.0017899999999997	F	F	F
0.7222200040000004	0.7777799959999996	0.1067200009999993	F	F	F
0.6662156308923322	0.6740449538844155	0.2193706731845465	T	T	T
0.9444299940000036	0.7222099900000032	0.0017899999999997	F	F	F
0.8888999819999981	0.7777900099999968	0.1066799979999971	F	F	F
0.8320122391128816	0.6674908520935708	0.2191308588969826	T	T	T
0.1111199999999997	0.8888800140000015	0.0018099999999990	F	F	F
0.0555500019999968	0.9444400069999972	0.1067000030000003	F	F	F
0.0002328873678070	0.8334909999191884	0.2112029094609731	T	T	T
0.2777599989999970	0.8888800140000015	0.0018099999999990	F	F	F
0.2222200040000004	0.9444400069999972	0.1067200009999993	F	F	F
0.1642474166162961	0.8299063135697218	0.2111114637809395	T	T	T
0.4444499909999990	0.8888999819999981	0.0018000000000029	F	F	F
0.3888899980000033	0.9444500210000015	0.1066899969999966	F	F	F
0.3314167221306649	0.8312476864430202	0.2116681922650303	T	T	T
0.6111199859999985	0.8888800140000015	0.0018099999999990	F	F	F
0.5555499789999985	0.9444500210000015	0.1066899969999966	F	F	F
0.4979186371695013	0.8316893487625127	0.2110309253492171	T	T	T
0.7777600289999995	0.8888800140000015	0.0018099999999990	F	F	F
0.7222200040000004	0.9444299940000036	0.1067200009999993	F	F	F
0.6653110924952879	0.8340465671367272	0.2095976196520526	T	T	T
0.9444500210000015	0.8888999819999981	0.0018000000000029	F	F	F
0.8888900279999987	0.9444500210000015	0.1067000030000003	F	F	F
0.8352905830973070	0.8361148440789463	0.2104693042640024	T	T	T
0.3862099950000015	0.0252100009999978	0.3365699949999978	F	F	F
0.6221731185075724	0.2437077045813594	0.3369433164743027	T	T	T
0.6537299749999974	0.0397999990000031	0.3406400080000012	F	F	F
0.4810299869999994	0.1689800019999979	0.3683600130000002	T	T	T
0.6999099849999979	0.1711699960000033	0.3778100010000003	T	T	T
0.5097600220000018	0.9990599750000015	0.3261699970000009	F	F	F
0.2878499930000018	0.0602600019999997	0.2814300060000008	F	F	F
0.7732499840000031	0.0595900009999966	0.2837100030000030	F	F	F
0.6486700179999971	0.9545300010000020	0.4026600119999983	F	F	F
0.3127700089999976	0.9412000180000035	0.4012300070000023	F	F	F
0.7032862864302838	0.3492549164621314	0.4069131983329253	T	T	T
0.7099285656661246	0.6829788076919262	0.3245855065134754	T	T	T
0.5995841862116654	0.6278549667157127	0.3236969703240148	T	T	T
0.5411167516451401	0.5168026214205529	0.3155487218686217	T	T	T
0.5948499559654714	0.4602479113109507	0.2990818454653492	T	T	T

0.7070915367233528	0.5164151891395609	0.3106902204918280	T	T	T
0.7654021085514037	0.6271059702749379	0.3216948675289670	T	T	T
0.7500438908205896	0.7626189726510527	0.3435752572805348	T	T	T
0.5592120326514898	0.6673951771944857	0.3424277336310372	T	T	T
0.4633138007678085	0.4754315554289547	0.3380906880429610	T	T	T
0.8407457443203253	0.6606033745699894	0.3477453382983371	T	T	T
0.6821917643357583	0.4009967537666532	0.4131436691848241	T	T	T
0.7472809725660863	0.4739677111724031	0.3230259763841382	T	T	T
0.3895241504617983	0.2847527616849130	0.2651908027619978	T	T	T

phenyl\_hy\_mo3o7\_ts

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14.9507999419999997 0.0000000000000000 0.0000000000000000

-7.4753999709999999 12.9477725567000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.0690994262999993

Ni Mo O C H

108 3 8 6 7

Selective dynamics

Direct

0.1111000100000012	0.0555500099999975	0.0018000000000029	F	F	F
0.0555500099999975	0.1111100099999973	0.1066900000000004	F	F	F
0.0014557599999989	0.0011441700000034	0.2110684399999982	T	T	T
0.2777900299999985	0.0555700000000030	0.0017899999999997	F	F	F
0.2222099999999969	0.1111000100000012	0.1066799999999972	F	F	F
0.1658205399999986	0.0001313699999983	0.2164356899999973	T	T	T
0.4444499800000017	0.0555500099999975	0.0018000000000029	F	F	F
0.3889000200000012	0.1111100099999973	0.1066799999999972	F	F	F
0.3331058600000034	0.9967067299999997	0.2105973299999988	T	T	T
0.6111000499999975	0.0555500099999975	0.0018000000000029	F	F	F
0.5555499999999967	0.1111100099999973	0.1066999999999965	F	F	F
0.4998507299999986	0.9999500200000000	0.2203216099999992	T	T	T
0.7777900099999968	0.0555700000000030	0.0017899999999997	F	F	F
0.7222099999999969	0.1111000100000012	0.1066799999999972	F	F	F
0.6633945600000004	0.9986399100000014	0.2117485699999975	T	T	T
0.9444500199999979	0.0555500099999975	0.0018000000000029	F	F	F
0.8888900199999981	0.1111000100000012	0.1066799999999972	F	F	F
0.8360020599999984	0.0006441800000019	0.2152511700000019	T	T	T
0.1111200100000005	0.2222400100000002	0.0018099999999990	F	F	F
0.0555599999999998	0.2777799999999999	0.1067200000000028	F	F	F
0.0036752700000022	0.1692055199999984	0.2110451400000031	T	T	T
0.2777900299999985	0.2222200200000017	0.0017899999999997	F	F	F
0.2222199899999993	0.2777799999999999	0.1067200000000028	F	F	F
0.1666486900000024	0.1692423100000013	0.2109526500000030	T	T	T
0.4444299999999970	0.2222100199999986	0.0017899999999997	F	F	F
0.3889000100000004	0.2777900199999976	0.1066799999999972	F	F	F
0.3385442100000020	0.1736087900000030	0.2155860100000027	T	T	T
0.6111200100000005	0.2222400100000002	0.0018099999999990	F	F	F
0.5555599999999998	0.2777799999999999	0.1067200000000028	F	F	F
0.5038784600000028	0.1711054700000005	0.2103911100000033	T	T	T
0.7777799899999991	0.2222100199999986	0.0017899999999997	F	F	F
0.7222200300000026	0.2777799999999999	0.1067200000000028	F	F	F
0.6669609300000019	0.1704645900000017	0.2117695000000026	T	T	T
0.9444299600000008	0.2222100199999986	0.0017899999999997	F	F	F
0.8888999500000025	0.2777900199999976	0.1066799999999972	F	F	F

0.8360081599999987	0.1711389800000021	0.2144006999999988	T	T	T
0.1111199999999997	0.3888800200000020	0.0018099999999990	F	F	F
0.0555600100000007	0.4444500199999979	0.1066900000000004	F	F	F
0.0014664199999999	0.3345616300000032	0.2113268900000023	T	T	T
0.2777600000000007	0.3888800200000020	0.0018099999999990	F	F	F
0.2222200200000017	0.4444400400000035	0.1067200000000028	F	F	F
0.1678807500000019	0.3350091399999968	0.2118235100000021	T	T	T
0.4444499800000017	0.3889000100000004	0.0018000000000029	F	F	F
0.3888900199999981	0.4444500199999979	0.1066900000000004	F	F	F
0.3342407499999993	0.3345207500000029	0.2110418500000009	T	T	T
0.6111199999999997	0.3888800200000020	0.0018099999999990	F	F	F
0.5555600400000031	0.4444500199999979	0.1066900000000004	F	F	F
0.5086861400000018	0.3431860299999983	0.2349448399999972	T	T	T
0.7777600200000023	0.3888800200000020	0.0018099999999990	F	F	F
0.7222200200000017	0.4444400400000035	0.1067200000000028	F	F	F
0.6699927000000017	0.3327299999999980	0.2127561499999970	T	T	T
0.9444500399999995	0.3889000100000004	0.0018000000000029	F	F	F
0.8888900399999997	0.4444500199999979	0.1066900000000004	F	F	F
0.8355778900000033	0.3349299300000013	0.2121868099999986	T	T	T
0.1110999899999996	0.5555499800000021	0.0018000000000029	F	F	F
0.0555499900000029	0.6111099999999965	0.1066900000000004	F	F	F
0.0011086800000015	0.5006001100000006	0.2117402399999975	T	T	T
0.2777900099999968	0.5555700099999967	0.0017899999999997	F	F	F
0.2222099999999969	0.6111000499999975	0.1066799999999972	F	F	F
0.1665257399999973	0.5001438399999998	0.2118145100000035	T	T	T
0.4444499700000009	0.5555499800000021	0.0018000000000029	F	F	F
0.3888900000000035	0.6111099999999965	0.1066799999999972	F	F	F
0.3320421000000024	0.5004447299999981	0.2109945400000015	T	T	T
0.6111000399999966	0.5555499800000021	0.0018000000000029	F	F	F
0.5555499900000029	0.6111099999999965	0.1066900000000004	F	F	F
0.4998709700000035	0.5046946200000022	0.2119985200000016	T	T	T
0.7777900099999968	0.5555700099999967	0.0017899999999997	F	F	F
0.7222099800000024	0.6111000499999975	0.1066799999999972	F	F	F
0.6716464799999997	0.5016687700000020	0.2082029600000013	T	T	T
0.9444500299999987	0.5555499800000021	0.0018000000000029	F	F	F
0.8888900000000035	0.6111099999999965	0.1066799999999972	F	F	F
0.8366056600000036	0.4999613600000004	0.2105051300000014	T	T	T
0.1111200200000013	0.7222400100000002	0.0018099999999990	F	F	F
0.0555599999999998	0.7777799999999999	0.1067200000000028	F	F	F
0.9998770699999966	0.6667672999999965	0.2114386100000019	T	T	T
0.2777900500000001	0.7222100400000002	0.0017899999999997	F	F	F
0.2222199899999993	0.7777799999999999	0.1067200000000028	F	F	F
0.1659792499999995	0.6657452600000013	0.2118418100000028	T	T	T
0.4444300099999978	0.7222200499999971	0.0017899999999997	F	F	F

0.3889000100000004	0.7777900099999968	0.1066799999999972	F	F	F
0.3318237399999973	0.6664642599999979	0.2115940799999976	T	T	T
0.6111200400000030	0.7222400100000002	0.0018099999999990	F	F	F
0.5555599999999998	0.7777799999999999	0.1067200000000028	F	F	F
0.4974743699999991	0.6687312399999996	0.2110581600000003	T	T	T
0.7777800300000024	0.7222200499999971	0.0017899999999997	F	F	F
0.7222199899999993	0.7777799999999999	0.1067200000000028	F	F	F
0.6670484300000012	0.6754306600000035	0.2185694799999993	T	T	T
0.9444300099999978	0.7222100400000002	0.0017899999999997	F	F	F
0.8888999500000025	0.7777900099999968	0.1066799999999972	F	F	F
0.8321359799999968	0.6668900900000025	0.2190026299999985	T	T	T
0.1111200599999975	0.8888800699999990	0.0018099999999990	F	F	F
0.0555499999999967	0.9444400100000010	0.1066999999999965	F	F	F
0.0004127600000032	0.8335359000000011	0.2112081900000007	T	T	T
0.2777600499999977	0.8888800699999990	0.0018099999999990	F	F	F
0.2222200100000009	0.9444400100000010	0.1067200000000028	F	F	F
0.1642963399999999	0.8297078900000017	0.2111478500000032	T	T	T
0.4444500199999979	0.8889000300000021	0.0018000000000029	F	F	F
0.3888900099999972	0.9444500299999987	0.1066900000000004	F	F	F
0.3314211900000004	0.8311310400000025	0.2117172299999979	T	T	T
0.6111200599999975	0.8888800699999990	0.0018099999999990	F	F	F
0.5555499999999967	0.9444500299999987	0.1066900000000004	F	F	F
0.4980013899999989	0.8321820099999968	0.2109832100000020	T	T	T
0.7777600800000002	0.8888800699999990	0.0018099999999990	F	F	F
0.7222200100000009	0.9444299999999970	0.1067200000000028	F	F	F
0.6656162700000010	0.8349505199999996	0.2094742000000025	T	T	T
0.9444500500000004	0.8889000300000021	0.0018000000000029	F	F	F
0.8888900099999972	0.9444500299999987	0.1066999999999965	F	F	F
0.8357497499999980	0.8365642799999975	0.2104348599999994	T	T	T
0.3862100200000000	0.0252100000000013	0.3365699900000010	F	F	F
0.6220086900000013	0.2422610899999995	0.3347921200000030	T	T	T
0.6537300299999984	0.0397999999999996	0.3406400000000005	F	F	F
0.4816168700000034	0.1682398399999983	0.3672502900000012	T	T	T
0.6944329100000033	0.1673375600000000	0.3780177100000017	T	T	T
0.5097600699999987	0.9990600400000034	0.3261699899999968	F	F	F
0.2878499799999972	0.0602600100000004	0.2814300000000003	F	F	F
0.7732499899999965	0.0595900000000000	0.2837099999999992	F	F	F
0.6486699900000019	0.9545300099999992	0.4026600099999982	F	F	F
0.3127700200000021	0.9412000599999999	0.4012300099999990	F	F	F
0.7025749499999989	0.3471607099999972	0.4057061600000011	T	T	T
0.7131938899999994	0.6843581199999988	0.3230568700000020	T	T	T
0.6031498199999987	0.6371061999999981	0.3224071599999974	T	T	T
0.5369022300000026	0.5265922199999977	0.3142591499999980	T	T	T
0.5836429499999980	0.4638788099999971	0.2968238999999997	T	T	T

0.6947888500000019	0.5103589900000003	0.3110384200000027	T	T	T
0.7606236800000019	0.6208304900000030	0.3206326500000003	T	T	T
0.7590739199999987	0.7638857299999984	0.3416930200000010	T	T	T
0.5689149999999970	0.6821876899999992	0.3418040999999974	T	T	T
0.4598584700000004	0.4907162599999992	0.3376910599999974	T	T	T
0.8355555099999989	0.6488504300000031	0.3464555300000001	T	T	T
0.6805287700000022	0.3974245599999975	0.4152408100000002	T	T	T
0.7282341299999970	0.4623943499999967	0.3250411100000008	T	T	T
0.4700744200000031	0.3301677099999978	0.3077476300000015	T	T	T

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Ni C O H  
108 6 1 6

Selective dynamics

Direct

0.1111000029999971	0.0555500019999968	0.0018000000000029	F	F	F
0.0555500019999968	0.1111100019999967	0.1066899969999966	F	F	F
-0.0005329841437689	-0.0000012467488876	0.2117315852117488	T	T	T
0.2777900099999968	0.0555699989999994	0.0017899999999997	F	F	F
0.2222100050000009	0.1111000029999971	0.1066799979999971	F	F	F
0.1651946797346125	-0.0014316527100392	0.2116951815427599	T	T	T
0.4444499909999990	0.0555500019999968	0.0018000000000029	F	F	F
0.3889000120000006	0.1111100019999967	0.1066799979999971	F	F	F
0.3321423539260487	-0.0020914219177893	0.2115958674664416	T	T	T
0.6111000180000019	0.0555500019999968	0.0018000000000029	F	F	F
0.5555499789999985	0.1111100019999967	0.1067000030000003	F	F	F
0.4995998653165399	-0.0012404389931363	0.2116316440024287	T	T	T
0.7777900099999968	0.0555699989999994	0.0017899999999997	F	F	F
0.7222099900000032	0.1111000029999971	0.1066799979999971	F	F	F
0.6663346098782704	0.0000209382101673	0.2117456436750079	T	T	T
0.9444500210000015	0.0555500019999968	0.0018000000000029	F	F	F
0.8888900279999987	0.1111000029999971	0.1066799979999971	F	F	F
0.8330232909209696	0.0003702634004084	0.2117262708838012	T	T	T
0.1111199999999997	0.2222400010000030	0.0018099999999990	F	F	F
0.0555599999999998	0.2777799959999996	0.1067200009999993	F	F	F
0.9991955293075088	0.1666621291434260	0.2117429661132614	T	T	T
0.2777900099999968	0.2222200040000004	0.0017899999999997	F	F	F
0.2222200040000004	0.2777799959999996	0.1067200009999993	F	F	F
0.1645096851227806	0.1654198721798625	0.2114734660113819	T	T	T
0.4444299939999965	0.2222100050000009	0.0017899999999997	F	F	F
0.3889000120000006	0.2777900099999968	0.1066799979999971	F	F	F
0.3287797950074930	0.1618967802426570	0.2102934426119678	T	T	T
0.6111199859999985	0.2222400010000030	0.0018099999999990	F	F	F
0.5555599930000028	0.2777799959999996	0.1067200009999993	F	F	F
0.4981291209853778	0.1627637891164883	0.2106272942975817	T	T	T
0.7777799959999996	0.2222100050000009	0.0017899999999997	F	F	F
0.7222200040000004	0.2777799959999996	0.1067200009999993	F	F	F
0.6662324111233084	0.1662795741180194	0.2111192281838024	T	T	T
0.9444299940000036	0.2222100050000009	0.0017899999999997	F	F	F
0.8888999819999981	0.2777900099999968	0.1066799979999971	F	F	F



0.8328013961554740	0.1668985261325932	0.2116354172258665	T	T	T
0.1111199999999997	0.3888800140000015	0.0018099999999990	F	F	F
0.0555599999999998	0.4444499909999990	0.1066899969999966	F	F	F
-0.0003674639695729	0.3333906060892391	0.2117371232327657	T	T	T
0.2777599989999970	0.3888800140000015	0.0018099999999990	F	F	F
0.2222200040000004	0.4444400069999972	0.1067200009999993	F	F	F
0.1654322691765739	0.3329913405516554	0.2118287049153248	T	T	T
0.4444499909999990	0.3889000120000006	0.0018000000000029	F	F	F
0.3888899980000033	0.4444499909999990	0.1066899969999966	F	F	F
0.3293713132373607	0.3312849844174846	0.2090564032697135	T	T	T
0.6111199859999985	0.3888800140000015	0.0018099999999990	F	F	F
0.5555599930000028	0.4444499909999990	0.1066899969999966	F	F	F
0.4929378282324274	0.3256327198354657	0.2178331129438440	T	T	T
0.7777600289999995	0.3888800140000015	0.0018099999999990	F	F	F
0.7222200040000004	0.4444400069999972	0.1067200009999993	F	F	F
0.6650735211569074	0.3336807025057799	0.2170432458248779	T	T	T
0.9444500210000015	0.3889000120000006	0.0018000000000029	F	F	F
0.8888900279999987	0.4444499909999990	0.1066899969999966	F	F	F
0.8332348598307234	0.3334334294876294	0.2111471090419994	T	T	T
0.1111000029999971	0.5555499789999985	0.0018000000000029	F	F	F
0.0555500019999968	0.6111099720000013	0.1066899969999966	F	F	F
0.0007574885197328	0.5000728943369955	0.2116072005859533	T	T	T
0.2777900099999968	0.5555700059999964	0.0017899999999997	F	F	F
0.2222100050000009	0.6111000180000019	0.1066799979999971	F	F	F
0.1666284386521929	0.4996369756751705	0.2117695991863569	T	T	T
0.4444499909999990	0.5555499789999985	0.0018000000000029	F	F	F
0.3888899980000033	0.6111099720000013	0.1066799979999971	F	F	F
0.3329309138619956	0.4996804900782454	0.2114034785380957	T	T	T
0.6111000180000019	0.5555499789999985	0.0018000000000029	F	F	F
0.5555499789999985	0.6111099720000013	0.1066899969999966	F	F	F
0.4998123466447409	0.4981442444046062	0.2175016656838004	T	T	T
0.7777900099999968	0.5555700059999964	0.0017899999999997	F	F	F
0.7222099900000032	0.6111000180000019	0.1066799979999971	F	F	F
0.6727399696681644	0.5060395930952682	0.2171879698444692	T	T	T
0.9444500210000015	0.5555499789999985	0.0018000000000029	F	F	F
0.8888900279999987	0.6111099720000013	0.1066799979999971	F	F	F
0.8363686687361466	0.5012406342256073	0.2105963852329234	T	T	T
0.1111199999999997	0.7222399710000005	0.0018099999999990	F	F	F
0.0555599999999998	0.7777799959999996	0.1067200009999993	F	F	F
0.0013787361294861	0.6673461981431409	0.2116082766828282	T	T	T
0.2777900099999968	0.7222099900000032	0.0017899999999997	F	F	F
0.2222200040000004	0.7777799959999996	0.1067200009999993	F	F	F
0.1671058328323230	0.6663608429950104	0.2117075281998675	T	T	T
0.4444299939999965	0.7222200040000004	0.0017899999999997	F	F	F

0.3889000120000006	0.7777900099999968	0.1066799979999971	F	F	F
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0.6111199859999985	0.7222399710000005	0.0018099999999990	F	F	F
0.5555599930000028	0.7777799959999996	0.1067200009999993	F	F	F
0.4997239292908008	0.6665303162147956	0.2111456296334315	T	T	T
0.7777799959999996	0.7222200040000004	0.0017899999999997	F	F	F
0.7222200040000004	0.7777799959999996	0.1067200009999993	F	F	F
0.6680125298327908	0.6695199423828850	0.2105918249153314	T	T	T
0.9444299940000036	0.7222099900000032	0.0017899999999997	F	F	F
0.8888999819999981	0.7777900099999968	0.1066799979999971	F	F	F
0.8370613846498931	0.6703836741139345	0.2102077128022923	T	T	T
0.1111199999999997	0.8888800140000015	0.0018099999999990	F	F	F
0.0555500019999968	0.9444400069999972	0.1067000030000003	F	F	F
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0.1666300845584220	0.8328428489162326	0.2117522839891554	T	T	T
0.4444499909999990	0.8888999819999981	0.0018000000000029	F	F	F
0.3888899980000033	0.9444500210000015	0.1066899969999966	F	F	F
0.3333627726005416	0.8325532372276516	0.2117181091244830	T	T	T
0.6111199859999985	0.8888800140000015	0.0018099999999990	F	F	F
0.5555499789999985	0.9444500210000015	0.1066899969999966	F	F	F
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0.7777600289999995	0.8888800140000015	0.0018099999999990	F	F	F
0.7222200040000004	0.9444299940000036	0.1067200009999993	F	F	F
0.6666994022815081	0.8339604666615318	0.2115972220655386	T	T	T
0.9444500210000015	0.8888999819999981	0.0018000000000029	F	F	F
0.8888900279999987	0.9444500210000015	0.1067000030000003	F	F	F
0.8340294648203086	0.8346878844108372	0.2116204987342153	T	T	T
0.6898971965719799	0.4687725776725017	0.3204954650721050	T	T	T
0.6353927096334619	0.5248171511651050	0.3198904125383493	T	T	T
0.5231899873528140	0.4717893584285495	0.3209057486003030	T	T	T
0.4693554113043996	0.3602408757308522	0.3262697984506484	T	T	T
0.5226940623091063	0.3035795857785751	0.3227756495894712	T	T	T
0.6346276011434646	0.3571554473843675	0.3201184184564035	T	T	T
0.3698152303411883	0.3075386525695408	0.3505970529315081	T	T	T
0.7708925436274110	0.5088789452424258	0.3366405338754780	T	T	T
0.6762443000005885	0.6057660263097592	0.3363347381774914	T	T	T
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0.4809142020527290	0.2230815185183519	0.3401462241823400	T	T	T
0.6730230245853132	0.3173752875716149	0.3420129382314427	T	T	T
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phenol\_ddo\_ni\_ts

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Ni C O H
108 6 1 6
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Selective dynamics

Direct

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0.2777900250000016	0.0555700029999997	0.0017899999999997	F	F	F
0.2222099950000000	0.1111000100000012	0.1066799990000007	F	F	F
0.1656220657222694	0.9986157858829724	0.2116377396367100	T	T	T
0.4444499829999984	0.0555500050000006	0.0018000000000029	F	F	F
0.3889000220000014	0.1111100090000008	0.1066799990000007	F	F	F
0.3324626553336416	0.9977396352174649	0.2116099108744670	T	T	T
0.6111000539999978	0.0555500050000006	0.0018000000000029	F	F	F
0.5555499970000000	0.1111100090000008	0.1067000039999968	F	F	F
0.4999808405279580	0.9986813137269259	0.2116806573624850	T	T	T
0.7777900090000003	0.0555700029999997	0.0017899999999997	F	F	F
0.7222099950000000	0.1111000100000012	0.1066799990000007	F	F	F
0.6668868000843682	0.0003114153301686	0.2117492185122321	T	T	T
0.9444500150000010	0.0555500050000006	0.0018000000000029	F	F	F
0.8888900150000012	0.1111000100000012	0.1066799990000007	F	F	F
0.8336922948174545	1.0007030570514783	0.2117735045419174	T	T	T
0.1111200080000003	0.2222400149999970	0.0018099999999990	F	F	F
0.0555599959999995	0.2777799990000034	0.1067199960000025	F	F	F
1.0001112471032847	0.1669486217733283	0.2115579319614322	T	T	T
0.2777900279999983	0.2222200180000016	0.0017899999999997	F	F	F
0.2222199939999996	0.2777799990000034	0.1067199960000025	F	F	F
0.1665996067017849	0.1667066751085969	0.2116969808277427	T	T	T
0.4444299970000003	0.2222100190000020	0.0017899999999997	F	F	F
0.3889000149999973	0.2777900159999973	0.1066799990000007	F	F	F
0.3293975190436174	0.1606801202429265	0.2097864103492250	T	T	T
0.6111200080000003	0.2222400149999970	0.0018099999999990	F	F	F
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0.4990607638814936	0.1620627975896592	0.2103469609454115	T	T	T
0.7777799899999991	0.2222100190000020	0.0017899999999997	F	F	F
0.7222200260000022	0.2777799990000034	0.1067199960000025	F	F	F
0.6669774057483052	0.1664683520313431	0.2113325307609098	T	T	T
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0.8334755516851456	0.1669405207286504	0.2116952039648392	T	T	T
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0.2222200180000016	0.4444400360000031	0.1067199960000025	F	F	F
0.1676747828957348	0.3335887826503767	0.2114284136807259	T	T	T
0.4444499760000014	0.3889000149999973	0.0018000000000029	F	F	F
0.3888900210000017	0.4444500159999976	0.1066900009999969	F	F	F
0.3375214615278581	0.3334783394069519	0.2372864665487273	T	T	T
0.6111199970000030	0.3888800180000018	0.0018099999999990	F	F	F
0.5555600420000033	0.4444500159999976	0.1066900009999969	F	F	F
0.4976326613152890	0.3269475415748467	0.2094011126672476	T	T	T
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0.7222200180000016	0.4444400360000031	0.1067199960000025	F	F	F
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0.6111000419999968	0.5555499800000021	0.0018000000000029	F	F	F
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0.7777900139999971	0.5555700139999971	0.0017899999999997	F	F	F
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0.6743032030088373	0.5071196401811608	0.2193814351339267	T	T	T
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0.6311863304799320	0.5273549240113469	0.3231704327585088	T	T	T
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