Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supplementary Information

General scaling relations and prediction of transition state energies in CHA/AlPO-34-structured zeolite catalysis related to the methanol-to-olefins conversion

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Table S1. Adsorption enthalpies of NH_3 and NH_2CH_3 in Me-CHA and Me-AlPO-34. The adsorption enthalpies of NH_3 calculated using hybrid functional with dispersion correction HSE06-D3 were included for comparison. The unit is kJ/mol.

	$\triangle H_{NH3}$		$\triangle H_{NH2CH3}$
XC functional	**BEEF-vdW**	**HSE06-D3**	**BEEF-vdW**
Si-AlPO-34	-104	-120	-145
Ge-AlPO-34	-94	-109	-134
Ti-AlPO-34	-78	-98	-119
Mg-AlPO-34	-142	-159	-184
Zn-AlPO-34	-127	-149	-169
Al-CHA	-125	-140	-167
Ga-CHA	-114	-131	-155

Note. The adsorption enthalpy differences between NH_3 and NH_2CH_3 in Me-CHA/AlPO-34 are 40 ~ 42 kJ/mol, agreeing well with the experimental results in H-ZSM-5 and H-MOR (40 kJ/mol, *J. Am. Chem. Soc.* 1996, *118,* 3262-3268).

Table S2. Definition of the relative TS enthalpies for each elementary step.

Elementary step	Calculation of the relative TS enthalpies
Concerted methylation of X	$\Delta H^{\neq} = H(TS) - H(HZ) - H(CH_3OH) - H(X)$
Stepwise methylation of X	$\Delta H^{\neq} = H(TS) + H(H_2O) - H(HZ) - H(CH_3OH) - H(X)$
Cyclization of diene	$\Delta H^{\neq} = H(TS) - H(HZ) - H(Diene)$
Hydride transfer to produce CH4	$\Delta H^{\neq} = H(TS) + H(H_2O) - H(HZ) - H(CH_3OH) - H(Olefin2)$
Hydride transfer to produce ethane or propane	$\Delta H^{\neq} = H(TS) - H(HZ) - H(Olefin1) - H(Olefin2)$
Ethylation of X	$\Delta H^{\neq} = H(TS) - H(HZ) - H(C_2H_4) - H(X)$
Elimination of propene in TME-cycle	$\Delta H^{\neq} = H(TS) + 2 * H(H_2O) - H(HZ) - 3 * H(CH_3OH) - H(TME)$
Elimination of propene in TMB-cycle	$\Delta H^{\neq} = H(TS) + 2 * H(H_2O) - H(HZ) - 3 * H(CH_3OH) - H(TMB)$

Note. HZ is zeolite; olefin1 is ethene or propene acting as hydride acceptor; olefin2 is hydride donor.

Table S3. The slopes in five representative scaling relations fitted using DFT calculated enthalpies with BEEF-vdW and HSE06-D3, respectively. The geometries of TS structures were optimized using BEEF-vdW functional.

Elementary reaction	**BEEF-vdW**	**HSE06-D3**
Concerted methylation (CH_3OH + C3)	1.07 ± 0.06	1.05 ± 0.05
Stepwise methylation (CH_3Z + C3)	0.74 ± 0.06	0.78 ± 0.06
Cyclization (C_6H_{10})	0.82 ± 0.06	0.85 ± 0.06
Hydride transfer (CH_3Z + C5-iso)	0.73 ± 0.05	0.77 ± 0.05
Ethylation (C_2H_5Z + C3)	0.85 ± 0.04	0.88 ± 0.04

Table S4. TS enthalpies in Al-CHA and Ga-CHA zeolites calculated and predicted using CHA or AlPO-34 optimized cell size.

	CHA cell size	**AlPO-34 cell size**	**Predicted data using scaling relations**	
			fitted in 5 Me-AlPO-34 zeotypes	**deduced from Bader charge and TS enthalpy in Si-AlPO-34**
Stepwise methylation of TMB				
Al-CHA	-26	-28	-33	-28
Ga-CHA	-17	-21	-23	-20
Elimination of propene from TME-cycle				
Al-CHA	-188	-196	-192	-194
Ga-CHA	-174	-184	-181	-184
Elimination of propene from TMB-cycle				
Al-CHA	-221	-233	-226	-228
Ga-CHA	-207	-221	-215	-218

Note. i) The calculated $\triangle H_{NH3}$ in Al-CHA and Ga-CHA using AlPO-34 cell size are -120 and -111 kJ/mol, respectively. ii) Cell parameter: CHA: 13.72, 13.72, and 14.86 Å; AlPO-34: 13.89, 13.89, and 15.09 Å.

Table S5. Bader charge variation of framework calculated in three systems for elementary steps or adsorption states of NH_2R.

		Si-AlPO-34	Mg-AlPO-34	Al-CHA
NH_2R adsorption				
1	NH_3	0.130	0.115	0.121
2	NH_2CH_3	0.115	0.104	0.110
Concerted methylation by CH_3OH				
3	C_2H_4	0.079	0.069	0.080
4	C_3H_6	0.083	0.072	0.082
5	C_4H_8-iso	0.091	0.083	0.091
6	TME	0.096	0.088	0.096
7	Toluene	0.086	0.076	0.084
8	TMB	0.092	0.079	0.091
9	CO	0.104	0.083	0.099
10	NH_3	0.098	0.092	0.098
Stepwise methylation by CH_3Z				
11	C_2H_4	0.205	0.203	0.214
12	C_3H_6	0.229	0.229	0.237
13	C_4H_8-iso	0.259	0.256	0.264
14	TME	0.266	0.267	0.277
15	Toluene	0.227	0.225	0.228
16	TMB	0.236	0.242	0.243
17	CO	0.261	0.247	0.248
18	H_2O	0.245	0.248	0.254
19	CH_3OH	0.259	0.265	0.267
20	NH_3	0.289	0.292	0.293
Cyclization				
21	C_6H_{10}	0.221	0.219	0.236
22	C_7H_{12}	0.245	0.241	0.258
Hydride Transfer				
23	CH_3Z + C4-1	0.245	0.240	0.251
24	CH_3Z + C5-iso	0.262	0.255	0.266
25	C_2H_5Z + C4-1	0.187	0.180	0.191
26	C_3H_7Z + C5-iso	0.108	0.112	0.125

Ethylation				
27	C_2H_5Z + C3	0.189	0.191	0.197
28	C_2H_5Z + C4-iso	0.218	0.217	0.225
29	C_2H_5Z + TME	0.236	0.227	0.240
C3 Elimination				
30	C3+TME	0.119	0.105	0.118
31	C3+TMB	0.119	0.103	0.113

Table S6. Calculated entropy contribution at 673 K of the three elementary steps Me-CHA and Me-AlPO-34. The unit is kJ/mol.

	Concerted methylation (CH3OH + C3)	**Hydride transfer** (CH3Z + C5-iso)	**Cyclization** (C6H10)
Si-AlPO-34	244	250	202
Ge-AlPO-34	242[a]	247	203
Ti-AlPO-34	244	247	200
Mg-AlPO-34	246	261[b]	203
Zn-AlPO-34	247	251	203
Al-CHA	243	247	202
Ga-CHA	243	246	202

Note. [a] There is one additional low imaginary frequency in the C3 methylation via converted pathway in all other systems except Ge-AlPO-34. This imaginary frequency was substituted by 12 cm^{-1} to calculate thermochemistry. [b] There is one low imaginary frequency in the hydride transfer between CH3Z and C5-iso in Mg-AlPO-34.

Equation S1. The relationship between the variation of Bader charge of framework and the Bader charge of organic species in ion pair TS structure.

For any ion-pair structure, including TS and intermediate,

$$Q_{Framework} = -Q_{Organic\ species}$$

For pure zeolite with acid site,

$$Q^{HZ}_{Framework} = -Q^{HZ}_{Proton} = -1$$

The variation of Bader charge of framework in TS of an elementary reaction,

$$\begin{aligned}\Delta Q_{Framework} &= Q^{TS}_{Framework} - Q^{HZ}_{Framework} \\ &= 1 + Q^{TS}_{Framework} \\ &= 1 - Q^{TS}_{Organic\ species}\end{aligned}$$

Note. Q is the calculated Bader charge data, and the Bader charge of the acidic proton is +1 in Me-CHA/AlPO-34 systems. The pure zeotypes (HZ) and gaseous reactants were employed as the reference for the analysis of Bader charge with consistency to the calculation of relative TS energies.

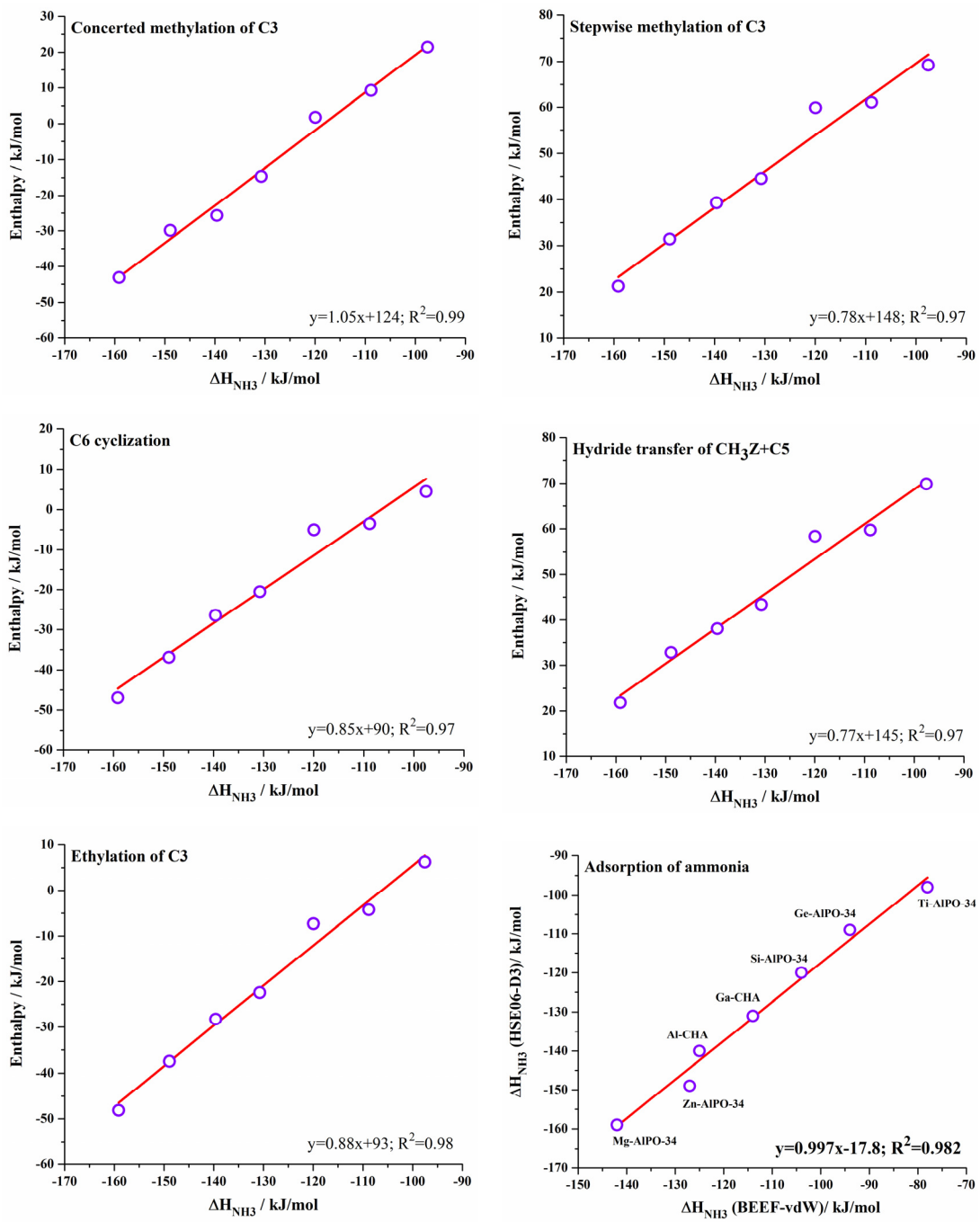

Figure S1. Scaling relations between the TS enthalpies and $\triangle H_{NH3}$ for five representative elementary reactions in Me-CHA/AlPO-34 calculated using HSE06-D3 functional. The agreement of the calculated adsorption enthalpies of NH_3 using BEEF-vdW and HSE06-D3 were included (See also Table S1).

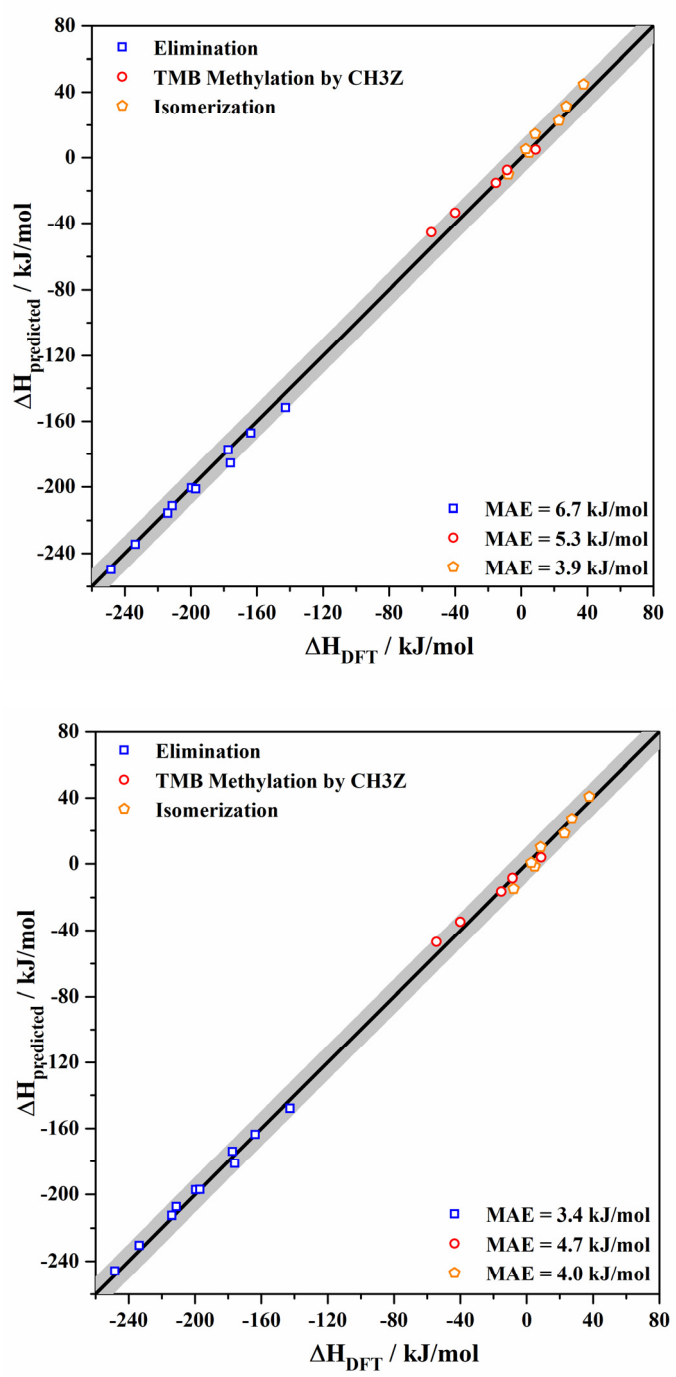

Figure S2. Using established Equation (2) and (3) to estimate the TS enthalpies for propene elimination and TMB stepwise methylation in Me-AlPO-34 and pentene isomerization in Me-CHA/AlPO-34 as testing elementary steps. The slope and intercept in the scaling relations were estimated using DFT calculated TS enthalpy and Bader charge in Si-AlPO-34 (top) or Ge-AlPO-34 (bottom) reference system. An interval of ±10 kJ/mol is shaded in grey around the diagonal line (y=x).

Optimized structures in Si-AlPO-34 in cif format

Ads-NH3-Si-AlPO-34

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H	H3	0.825275	0.628768	0.640996
H	H4	0.816349	0.743359	0.620451
N	N5	0.802066	0.668380	0.596077
O	O6	0.073723	0.290514	0.502239
O	O7	0.296535	0.398435	0.839652
O	O8	0.823634	0.437045	0.618277
O	O9	0.486675	0.153742	0.459870
O	O10	0.728368	0.619463	0.824581
O	O11	0.965566	0.729413	0.165403
O	O12	0.491403	0.762721	0.955742
O	O13	0.145508	0.476866	0.800630
O	O14	0.402799	0.954474	0.163038
O	O15	0.620324	0.059738	0.515696
O	O16	0.157955	0.099064	0.286206
O	O17	0.821523	0.814495	0.122789
O	O18	0.714510	0.292371	0.502513
O	O19	0.599370	0.415150	0.839509
O	O20	0.562083	0.900105	0.621800
O	O21	0.847934	0.854411	0.467501
O	O22	0.374489	0.632068	0.833861
O	O23	0.268392	0.750766	0.174146
O	O24	0.239810	0.247717	0.954557

O	O25	0.518212	0.185982	0.798472
O	O26	0.046035	0.962458	0.165254
O	O27	0.933535	0.088923	0.514816
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O	O29	0.188147	0.521443	0.130768
O	O30	0.699970	0.935778	0.500311
O	O31	0.578530	0.702589	0.837267
O	O32	0.093784	0.175370	0.621617
O	O33	0.147107	0.517419	0.463463
O	O34	0.365986	0.264528	0.828457
O	O35	0.250113	0.034956	0.175282
O	O36	0.756194	0.513339	0.948988
O	O37	0.809287	0.846963	0.794581
O	O38	0.035372	0.594941	0.166188
O	O39	0.918998	0.368612	0.514106
O	O40	0.420181	0.844036	0.288006
O	O41	0.479560	0.182423	0.128144
O	O42	0.909353	0.709715	0.440229
O	O43	0.691614	0.612488	0.084909
O	O44	0.168680	0.581091	0.306693
O	O45	0.500711	0.862045	0.464405
O	O46	0.584757	0.057299	0.755368
O	O47	0.359732	0.952136	0.421416
O	O48	0.824185	0.908118	0.639175
O	O49	0.165867	0.197291	0.801227
O	O50	0.253607	0.389153	0.097630
O	O51	0.020968	0.279297	0.748991
O	O52	0.491479	0.245128	0.972000
O	O53	0.839159	0.528265	0.126055
O	O54	0.272654	0.716832	0.429294
O	O55	0.387445	0.592602	0.086076
O	O56	0.422347	0.100972	0.304726
O	O57	0.130386	0.152764	0.463197
O	O58	0.939019	0.045762	0.758507
O	O59	0.057737	0.924623	0.417711
O	O60	0.091456	0.439591	0.641672
O	O61	0.798424	0.492028	0.791145
O	O62	0.611429	0.379296	0.089770
O	O63	0.716613	0.261379	0.748940
O	O64	0.746800	0.762350	0.970367
O	O65	0.468659	0.821284	0.133451
O	O66	0.289501	0.086991	0.425000
O	O67	0.407410	0.311090	0.087822
O	O68	0.892174	0.820535	0.301776

O	O69	0.840795	0.487197	0.458506
O	O70	0.950482	0.412661	0.758516
O	O71	0.067949	0.637111	0.415234
O	O72	0.558590	0.173779	0.639908
O	O73	0.505269	0.831152	0.801326
O	O74	0.620636	0.745283	0.096117
O	O75	0.734489	0.973161	0.752217
O	O76	0.232090	0.499770	0.975038
O	O77	0.176455	0.159828	0.128940
Al	Al78	0.930408	0.606406	0.396214
Al	Al79	0.596066	0.940274	0.732740
Al	Al80	0.268469	0.275792	0.068084
Al	Al81	0.387967	0.844173	0.400430
Al	Al82	0.055414	0.174441	0.732395
Al	Al83	0.725366	0.508583	0.063432
Al	Al84	0.154915	0.061095	0.398761
Al	Al85	0.822559	0.398444	0.730270
Al	Al86	0.492220	0.731168	0.068656
Al	Al87	0.058860	0.404169	0.529235
Al	Al88	0.715459	0.733661	0.858845
Al	Al89	0.388091	0.068294	0.192722
Al	Al90	0.593496	0.168951	0.528597
Al	Al91	0.262227	0.502064	0.862287
Al	Al92	0.930908	0.833094	0.193080
Al	Al93	0.828842	0.948513	0.525448
Al	Al94	0.492824	0.277179	0.859934
Al	Al95	0.164620	0.612322	0.194465
Si	Si96	0.928346	0.831052	0.404294
P	P97	0.057772	0.175863	0.524939
P	P98	0.719982	0.509071	0.852588
P	P99	0.389646	0.842424	0.189997
P	P100	0.825278	0.395964	0.522817
P	P101	0.487370	0.732048	0.857724
P	P102	0.157166	0.063479	0.189946
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P	P105	0.935171	0.609334	0.185747
P	P106	0.594584	0.169530	0.735333
P	P107	0.265720	0.501101	0.072252
P	P108	0.163717	0.613232	0.403236
P	P109	0.826687	0.944698	0.735990
P	P110	0.497105	0.279485	0.069568
P	P111	0.388329	0.072703	0.402281
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P	P113	0.720613	0.733722	0.069232

Ads-CH3NH2-Si-AlPO-34

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H	H5	0.654506	0.642297	0.533679
H	H6	0.631184	0.579964	0.641384
C	C7	0.677450	0.596669	0.579602
N	N8	0.799221	0.666547	0.598203
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O	O23	0.562316	0.901153	0.621831
O	O24	0.847620	0.853908	0.467605

O	O25	0.374839	0.631745	0.833065
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O	O27	0.239371	0.247166	0.954303
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O	O29	0.045992	0.962502	0.165193
O	O30	0.933478	0.088801	0.514239
O	O31	0.899862	0.578911	0.282826
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O	O33	0.699678	0.934715	0.500445
O	O34	0.578873	0.702401	0.836381
O	O35	0.093362	0.175150	0.621395
O	O36	0.147097	0.517184	0.463302
O	O37	0.366205	0.264586	0.828529
O	O38	0.250119	0.035200	0.174670
O	O39	0.755448	0.512602	0.949062
O	O40	0.809653	0.847012	0.794451
O	O41	0.035571	0.595367	0.165413
O	O42	0.918671	0.367828	0.514011
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O	O44	0.479532	0.182448	0.127990
O	O45	0.909381	0.709588	0.439232
O	O46	0.691581	0.612757	0.084791
O	O47	0.168138	0.580532	0.306428
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O	O62	0.057446	0.924590	0.417460
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O	O64	0.798566	0.491979	0.791274
O	O65	0.611128	0.379673	0.090453
O	O66	0.716696	0.261622	0.748157
O	O67	0.746389	0.762638	0.970342
O	O68	0.468452	0.821428	0.132838

O	O69	0.289439	0.086753	0.425262
O	O70	0.407004	0.310750	0.087483
O	O71	0.891590	0.821237	0.301703
O	O72	0.841040	0.486810	0.458090
O	O73	0.950629	0.412637	0.758531
O	O74	0.068202	0.637132	0.415291
O	O75	0.558038	0.172216	0.639788
O	O76	0.505418	0.830986	0.801099
O	O77	0.620617	0.745545	0.096345
O	O78	0.734619	0.973135	0.752564
O	O79	0.232553	0.500508	0.974748
O	O80	0.176064	0.159953	0.128941
Al	Al81	0.930618	0.606493	0.396053
Al	Al82	0.596371	0.940553	0.732910
Al	Al83	0.268097	0.275574	0.067803
Al	Al84	0.388116	0.844012	0.400151
Al	Al85	0.055477	0.174421	0.732257
Al	Al86	0.725148	0.508678	0.063554
Al	Al87	0.154846	0.060881	0.398671
Al	Al88	0.822897	0.398735	0.730085
Al	Al89	0.492191	0.731120	0.068445
Al	Al90	0.058740	0.403924	0.529026
Al	Al91	0.715829	0.733920	0.858802
Al	Al92	0.387939	0.068351	0.192577
Al	Al93	0.593581	0.168526	0.528450
Al	Al94	0.262392	0.502098	0.862026
Al	Al95	0.930712	0.833291	0.193214
Al	Al96	0.829063	0.948331	0.525430
Al	Al97	0.493190	0.277525	0.859845
Al	Al98	0.164460	0.612258	0.194257
Si	Si99	0.928034	0.830669	0.404192
P	P100	0.057679	0.175714	0.524622
P	P101	0.720029	0.509069	0.852542
P	P102	0.389718	0.842486	0.189853
P	P103	0.825526	0.395998	0.522790
P	P104	0.487629	0.731700	0.857173
P	P105	0.157120	0.063554	0.189778
P	P106	0.596014	0.939578	0.525362
P	P107	0.266862	0.277021	0.856332
P	P108	0.935228	0.609345	0.185596
P	P109	0.594688	0.169398	0.735286
P	P110	0.265776	0.501266	0.072006
P	P111	0.163678	0.612955	0.402999
P	P112	0.826973	0.944948	0.736110

P	P113	0.497149	0.279677	0.069603
P	P114	0.388208	0.072512	0.402208
P	P115	0.052534	0.401618	0.736963
P	P116	0.720547	0.734006	0.069239

TS-Methylation-MeOH-C2-Si-AlPO-34

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H	H3	0.647292	0.489202	0.548178
H	H4	0.605993	0.598501	0.545186
H	H5	0.802752	0.732441	0.619535
H	H6	0.452369	0.346369	0.647071
H	H7	0.412110	0.454863	0.647618
H	H8	0.468368	0.357722	0.483360
H	H9	0.427744	0.466242	0.482760
C	C10	0.612815	0.534517	0.580373
C	C11	0.439911	0.406398	0.610240
C	C12	0.448071	0.412222	0.520444
O	O13	0.079577	0.293551	0.503780
O	O14	0.298960	0.400572	0.839450
O	O15	0.821002	0.428568	0.619092
O	O16	0.486409	0.158312	0.463419
O	O17	0.729092	0.619499	0.828533
O	O18	0.966405	0.730427	0.169348
O	O19	0.492910	0.760863	0.957479
O	O20	0.147328	0.478371	0.802034
O	O21	0.404225	0.955872	0.166815

O	O22	0.611950	0.055780	0.521890
O	O23	0.160268	0.101535	0.288435
O	O24	0.824243	0.816621	0.122498
O	O25	0.715863	0.288832	0.500028
O	O26	0.599565	0.415803	0.838388
O	O27	0.565017	0.895716	0.624574
O	O28	0.848222	0.858610	0.467701
O	O29	0.375994	0.633310	0.834082
O	O30	0.269010	0.752352	0.177899
O	O31	0.243231	0.251762	0.956367
O	O32	0.518562	0.186014	0.801537
O	O33	0.047267	0.963311	0.168377
O	O34	0.937015	0.092265	0.518329
O	O35	0.900982	0.578943	0.285882
O	O36	0.189944	0.524061	0.132285
O	O37	0.702755	0.942560	0.500618
O	O38	0.579619	0.703015	0.836480
O	O39	0.098836	0.179320	0.624142
O	O40	0.150392	0.519317	0.465820
O	O41	0.368381	0.266580	0.829793
O	O42	0.251553	0.036697	0.177554
O	O43	0.752371	0.509836	0.952103
O	O44	0.809717	0.849498	0.796546
O	O45	0.035890	0.595872	0.167530
O	O46	0.920923	0.367864	0.513060
O	O47	0.422683	0.844739	0.290467
O	O48	0.480680	0.183364	0.130693
O	O49	0.905639	0.709019	0.439842
O	O50	0.692319	0.614455	0.086681
O	O51	0.168066	0.581762	0.309036
O	O52	0.500825	0.858945	0.467597
O	O53	0.582758	0.057720	0.751312
O	O54	0.365310	0.955556	0.424389
O	O55	0.821935	0.912192	0.641213
O	O56	0.168120	0.198834	0.803279
O	O57	0.253766	0.390085	0.100533
O	O58	0.023148	0.280662	0.751374
O	O59	0.494129	0.249314	0.975424
O	O60	0.839482	0.529891	0.128794
O	O61	0.272567	0.718866	0.430610
O	O62	0.389338	0.593229	0.089200
O	O63	0.423615	0.103886	0.307688
O	O64	0.133509	0.153549	0.466054
O	O65	0.940712	0.047498	0.760216

O	O66	0.056497	0.923468	0.417465
O	O67	0.093067	0.439809	0.643140
O	O68	0.799878	0.490701	0.796092
O	O69	0.611438	0.381455	0.095546
O	O70	0.717812	0.261826	0.753555
O	O71	0.744872	0.763582	0.971597
O	O72	0.468311	0.821798	0.134752
O	O73	0.288973	0.085980	0.427752
O	O74	0.407290	0.311411	0.091822
O	O75	0.889290	0.821985	0.302976
O	O76	0.839800	0.484944	0.459978
O	O77	0.951995	0.413543	0.759925
O	O78	0.067060	0.636200	0.419133
O	O79	0.561882	0.184043	0.642105
O	O80	0.507133	0.833496	0.804595
O	O81	0.622518	0.747954	0.099699
O	O82	0.736430	0.977690	0.757015
O	O83	0.235236	0.501234	0.976953
O	O84	0.176599	0.160341	0.130594
O	O85	0.794650	0.661371	0.602318
Al	Al86	0.929302	0.606755	0.399911
Al	Al87	0.597776	0.941567	0.734822
Al	Al88	0.268980	0.276977	0.070615
Al	Al89	0.389820	0.845015	0.402810
Al	Al90	0.057019	0.175569	0.734570
Al	Al91	0.725499	0.509888	0.066451
Al	Al92	0.153920	0.059582	0.400464
Al	Al93	0.823772	0.399699	0.732196
Al	Al94	0.493742	0.732026	0.070970
Al	Al95	0.060493	0.405144	0.530497
Al	Al96	0.717088	0.734701	0.859563
Al	Al97	0.389194	0.069651	0.195559
Al	Al98	0.593485	0.170043	0.531255
Al	Al99	0.263786	0.503778	0.863925
Al	Al100	0.931051	0.834014	0.195437
Al	Al101	0.830224	0.951517	0.527479
Al	Al102	0.494957	0.278614	0.863067
Al	Al103	0.164812	0.613543	0.196742
Si	Si104	0.925873	0.830286	0.405653
P	P105	0.061381	0.178114	0.527465
P	P106	0.720706	0.508967	0.854765
P	P107	0.390668	0.843337	0.192747
P	P108	0.825733	0.393209	0.523079
P	P109	0.489160	0.732798	0.858912

P	P110	0.158172	0.064665	0.192254
P	P111	0.595485	0.938283	0.528625
P	P112	0.269154	0.279380	0.858065
P	P113	0.935779	0.610068	0.188777
P	P114	0.595878	0.172401	0.737095
P	P115	0.267416	0.502608	0.074652
P	P116	0.163626	0.614269	0.405683
P	P117	0.827174	0.947343	0.738335
P	P118	0.498168	0.281478	0.073490
P	P119	0.389574	0.074559	0.405137
P	P120	0.053815	0.402702	0.738758
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TS-Methylation-MeOH-C3-Si-AlPO-34

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H	H2	0.620254	0.543523	0.656537
H	H3	0.649214	0.493760	0.550926
H	H4	0.608873	0.603406	0.548891
H	H5	0.802745	0.735046	0.617186
H	H6	0.461948	0.357493	0.639834
H	H7	0.419523	0.464373	0.641393
H	H8	0.455934	0.351611	0.479071
H	H9	0.320618	0.411235	0.424055
H	H10	0.458067	0.515603	0.403941
H	H11	0.382919	0.529357	0.494922
C	C12	0.620985	0.543280	0.585067
C	C13	0.446778	0.415900	0.603265

C	C14	0.435810	0.408510	0.513301
C	C15	0.398256	0.471223	0.457169
O	O16	0.079920	0.293753	0.504422
O	O17	0.299013	0.400456	0.840446
O	O18	0.821166	0.427667	0.619484
O	O19	0.486100	0.157516	0.463791
O	O20	0.728435	0.618981	0.828305
O	O21	0.966940	0.729998	0.169828
O	O22	0.493170	0.761848	0.958003
O	O23	0.147075	0.477616	0.802466
O	O24	0.404544	0.955354	0.167051
O	O25	0.612469	0.055933	0.521104
O	O26	0.159674	0.100873	0.288669
O	O27	0.824468	0.815773	0.122738
O	O28	0.715664	0.288959	0.499769
O	O29	0.599463	0.415374	0.840160
O	O30	0.564476	0.896189	0.624616
O	O31	0.847643	0.858025	0.467796
O	O32	0.375443	0.633284	0.835391
O	O33	0.269298	0.751760	0.177627
O	O34	0.242899	0.251114	0.956766
O	O35	0.518031	0.185643	0.801275
O	O36	0.047907	0.962950	0.168087
O	O37	0.937021	0.092148	0.517293
O	O38	0.900953	0.578495	0.286289
O	O39	0.190420	0.523222	0.133394
O	O40	0.702494	0.941924	0.501029
O	O41	0.579130	0.702607	0.837478
O	O42	0.097613	0.177864	0.624242
O	O43	0.150150	0.518846	0.466247
O	O44	0.367844	0.265985	0.830170
O	O45	0.252105	0.036483	0.178373
O	O46	0.754270	0.511169	0.952024
O	O47	0.809072	0.848881	0.796482
O	O48	0.036076	0.595099	0.168249
O	O49	0.920542	0.367257	0.512674
O	O50	0.421929	0.843868	0.290990
O	O51	0.481237	0.183009	0.130951
O	O52	0.905539	0.708976	0.440063
O	O53	0.692374	0.613606	0.087081
O	O54	0.168944	0.581940	0.309637
O	O55	0.500780	0.858739	0.467643
O	O56	0.582527	0.057196	0.752457
O	O57	0.364325	0.954854	0.424645

O	O58	0.822598	0.912198	0.641169
O	O59	0.167657	0.198923	0.803750
O	O60	0.254856	0.389955	0.101084
O	O61	0.022541	0.280164	0.751108
O	O62	0.493051	0.247194	0.975286
O	O63	0.839843	0.529485	0.129092
O	O64	0.272734	0.718372	0.431738
O	O65	0.389613	0.593167	0.089173
O	O66	0.424318	0.103406	0.307947
O	O67	0.134128	0.154414	0.465942
O	O68	0.940392	0.047111	0.760707
O	O69	0.056417	0.923722	0.418697
O	O70	0.092177	0.439963	0.643602
O	O71	0.799120	0.490338	0.795618
O	O72	0.612210	0.380501	0.094200
O	O73	0.717619	0.261234	0.754441
O	O74	0.745365	0.762697	0.971780
O	O75	0.469072	0.821427	0.135747
O	O76	0.289151	0.086220	0.427302
O	O77	0.408122	0.311222	0.091834
O	O78	0.890365	0.822595	0.303100
O	O79	0.840182	0.485387	0.460773
O	O80	0.951641	0.413182	0.760953
O	O81	0.067293	0.636247	0.419301
O	O82	0.562588	0.183088	0.642280
O	O83	0.506813	0.832939	0.804612
O	O84	0.622811	0.747334	0.099669
O	O85	0.736128	0.977189	0.756592
O	O86	0.234589	0.500426	0.977685
O	O87	0.177495	0.160282	0.131027
O	O88	0.795452	0.663778	0.601479
Al	Al89	0.929392	0.606655	0.400251
Al	Al90	0.597383	0.941198	0.735021
Al	Al91	0.269720	0.276721	0.070734
Al	Al92	0.389471	0.844734	0.403305
Al	Al93	0.056746	0.175204	0.734830
Al	Al94	0.726160	0.509514	0.066247
Al	Al95	0.153961	0.059600	0.400815
Al	Al96	0.823369	0.398945	0.732678
Al	Al97	0.494166	0.731981	0.071215
Al	Al98	0.059926	0.404861	0.531076
Al	Al99	0.716685	0.734165	0.859764
Al	Al100	0.389824	0.069332	0.195841
Al	Al101	0.593613	0.169991	0.531278

Al	Al102	0.263505	0.503311	0.864577
Al	Al103	0.931664	0.833777	0.195450
Al	Al104	0.830235	0.951504	0.527432
Al	Al105	0.494352	0.277934	0.863035
Al	Al106	0.165203	0.613103	0.197194
Si	Si107	0.926029	0.830467	0.405936
P	P108	0.061280	0.177933	0.527522
P	P109	0.720667	0.508829	0.855001
P	P110	0.390824	0.842796	0.193087
P	P111	0.825574	0.392917	0.523252
P	P112	0.488860	0.732732	0.859578
P	P113	0.158582	0.064339	0.192501
P	P114	0.595407	0.938305	0.528624
P	P115	0.268959	0.279143	0.858449
P	P116	0.936023	0.609536	0.189196
P	P117	0.595757	0.171819	0.737531
P	P118	0.267711	0.502152	0.075144
P	P119	0.163780	0.614110	0.406271
P	P120	0.827031	0.946983	0.738394
P	P121	0.498477	0.280588	0.073119
P	P122	0.389550	0.074193	0.405292
P	P123	0.053333	0.402332	0.739246
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TS-Methylation-MeOH-C4-iso-Si-AlPO-34

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H	H6	0.397552	0.550510	0.368344
H	H7	0.541706	0.638155	0.380499
H	H8	0.449941	0.633140	0.465482
H	H9	0.507831	0.356946	0.434268
H	H10	0.563533	0.466890	0.354455
H	H11	0.420440	0.370167	0.355588
H	H12	0.450929	0.395211	0.576706
H	H13	0.431037	0.516692	0.589537
C	C14	0.639562	0.576275	0.571937
C	C15	0.458387	0.470623	0.548514
C	C16	0.471364	0.489255	0.458989
C	C17	0.465164	0.583767	0.417290
C	C18	0.493214	0.416783	0.398647
O	O19	0.069023	0.284479	0.509307
O	O20	0.291544	0.392570	0.846261
O	O21	0.814902	0.423226	0.624834
O	O22	0.479223	0.147414	0.468699
O	O23	0.724169	0.613488	0.834725
O	O24	0.958949	0.723099	0.174255
O	O25	0.486054	0.751968	0.963079
O	O26	0.140507	0.471089	0.807347
O	O27	0.396862	0.948381	0.173788
O	O28	0.609927	0.050140	0.524586
O	O29	0.156450	0.096710	0.294098
O	O30	0.816784	0.809853	0.128615
O	O31	0.708072	0.282734	0.506363
O	O32	0.592776	0.409944	0.845624
O	O33	0.554835	0.890758	0.630489
O	O34	0.838950	0.848054	0.473551
O	O35	0.369217	0.625638	0.839163
O	O36	0.261754	0.744614	0.183067
O	O37	0.233852	0.242381	0.961775
O	O38	0.512951	0.180327	0.806859
O	O39	0.039190	0.956234	0.176823
O	O40	0.927899	0.082718	0.521842
O	O41	0.893068	0.572943	0.291884
O	O42	0.181538	0.515805	0.137235
O	O43	0.692984	0.928977	0.508627
O	O44	0.573070	0.695591	0.841525
O	O45	0.088008	0.169184	0.629079
O	O46	0.143375	0.510545	0.470663

O	O47	0.360375	0.257999	0.836281
O	O48	0.243589	0.028741	0.181945
O	O49	0.746205	0.503640	0.958497
O	O50	0.803476	0.842458	0.803300
O	O51	0.028332	0.588442	0.174329
O	O52	0.913301	0.361376	0.518348
O	O53	0.415760	0.835061	0.295608
O	O54	0.473042	0.175723	0.135770
O	O55	0.902216	0.703149	0.447381
O	O56	0.685451	0.607242	0.093928
O	O57	0.162663	0.573652	0.313991
O	O58	0.493040	0.852396	0.473132
O	O59	0.577487	0.050835	0.761447
O	O60	0.355330	0.946202	0.427036
O	O61	0.818577	0.904000	0.647403
O	O62	0.160692	0.191462	0.808165
O	O63	0.246246	0.382414	0.105681
O	O64	0.015791	0.273669	0.756250
O	O65	0.487313	0.242699	0.980639
O	O66	0.831826	0.521964	0.135128
O	O67	0.266203	0.710077	0.436039
O	O68	0.381614	0.585740	0.096384
O	O69	0.414976	0.097871	0.312962
O	O70	0.125280	0.146572	0.470964
O	O71	0.933306	0.040704	0.767041
O	O72	0.048174	0.917769	0.421516
O	O73	0.085714	0.433191	0.648395
O	O74	0.792858	0.483101	0.802634
O	O75	0.603318	0.374321	0.101648
O	O76	0.711627	0.254827	0.758038
O	O77	0.736064	0.755462	0.978156
O	O78	0.461037	0.814989	0.139219
O	O79	0.281449	0.078102	0.434516
O	O80	0.399034	0.303272	0.097290
O	O81	0.879263	0.810212	0.308988
O	O82	0.832404	0.478470	0.465509
O	O83	0.945263	0.407059	0.765568
O	O84	0.060724	0.627886	0.423410
O	O85	0.554432	0.171061	0.647847
O	O86	0.500225	0.825832	0.810626
O	O87	0.614592	0.739834	0.106984
O	O88	0.728866	0.968550	0.760334
O	O89	0.229359	0.495126	0.982277
O	O90	0.168209	0.152423	0.135954

O	O91	0.805913	0.664185	0.612594
Al	Al92	0.923188	0.599594	0.405677
Al	Al93	0.590236	0.934272	0.741054
Al	Al94	0.260697	0.268752	0.075511
Al	Al95	0.382092	0.837136	0.407598
Al	Al96	0.049574	0.168447	0.739943
Al	Al97	0.718048	0.502351	0.072460
Al	Al98	0.147495	0.053674	0.406088
Al	Al99	0.816885	0.393023	0.737803
Al	Al100	0.486245	0.724142	0.076636
Al	Al101	0.052515	0.397417	0.536090
Al	Al102	0.710124	0.727250	0.865771
Al	Al103	0.381391	0.062365	0.200895
Al	Al104	0.587056	0.161897	0.536694
Al	Al105	0.257040	0.496158	0.869004
Al	Al106	0.923153	0.826067	0.201555
Al	Al107	0.822658	0.942179	0.533660
Al	Al108	0.488055	0.272283	0.867892
Al	Al109	0.157535	0.605787	0.201970
Si	Si110	0.918466	0.822399	0.411226
P	P111	0.052032	0.169474	0.532376
P	P112	0.714116	0.502259	0.861055
P	P113	0.383440	0.835517	0.198124
P	P114	0.818238	0.386861	0.528966
P	P115	0.482299	0.724728	0.864272
P	P116	0.151149	0.057721	0.198143
P	P117	0.588055	0.930966	0.534323
P	P118	0.261389	0.271219	0.863611
P	P119	0.928185	0.602873	0.194644
P	P120	0.589604	0.164516	0.743388
P	P121	0.259964	0.495085	0.080082
P	P122	0.157245	0.605709	0.410638
P	P123	0.820967	0.939658	0.744266
P	P124	0.490441	0.274000	0.078670
P	P125	0.381469	0.066392	0.410332
P	P126	0.046790	0.395859	0.744069
P	P127	0.713940	0.728210	0.077328

TS-Methylation-MeOH-C6-Si-AlPO-34

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H	H2	0.613645	0.573210	0.629697
H	H3	0.657800	0.515842	0.536785
H	H4	0.655953	0.648598	0.521589
H	H5	0.815436	0.733898	0.629411
H	H6	0.399703	0.551255	0.374256
H	H7	0.545067	0.636224	0.380153
H	H8	0.459652	0.641834	0.465231
H	H9	0.526266	0.369859	0.433747
H	H10	0.559394	0.474079	0.352504
H	H11	0.421045	0.366199	0.366184
H	H12	0.467410	0.373567	0.659620
H	H13	0.458472	0.313116	0.554003
H	H14	0.339099	0.301800	0.604583
H	H15	0.317046	0.493382	0.601643
H	H16	0.447729	0.615828	0.598754
H	H17	0.418305	0.514404	0.681458
C	C18	0.428515	0.357790	0.594071
C	C19	0.406430	0.526599	0.611604
C	C20	0.640845	0.578392	0.562115
C	C21	0.445717	0.464405	0.553107
C	C22	0.474727	0.492102	0.465301
C	C23	0.470494	0.586750	0.420394
C	C24	0.497982	0.421853	0.402262
O	O25	0.069481	0.284660	0.509442
O	O26	0.291944	0.392904	0.846472
O	O27	0.815359	0.422954	0.624894
O	O28	0.479930	0.145946	0.468535
O	O29	0.723536	0.612988	0.835220
O	O30	0.959262	0.723158	0.174608
O	O31	0.485962	0.752478	0.963267
O	O32	0.140624	0.470853	0.806959

O	O33	0.396709	0.948257	0.173004
O	O34	0.612569	0.050871	0.525286
O	O35	0.157249	0.097425	0.294086
O	O36	0.816828	0.809597	0.128744
O	O37	0.707723	0.283296	0.506137
O	O38	0.592534	0.409323	0.846010
O	O39	0.555241	0.890304	0.630409
O	O40	0.840940	0.848851	0.473893
O	O41	0.368808	0.625647	0.839654
O	O42	0.261607	0.744560	0.182994
O	O43	0.232905	0.242243	0.961817
O	O44	0.512345	0.179857	0.806461
O	O45	0.039258	0.956427	0.177210
O	O46	0.928131	0.082956	0.522167
O	O47	0.893470	0.572659	0.291977
O	O48	0.181614	0.515702	0.137543
O	O49	0.693062	0.927668	0.508365
O	O50	0.572529	0.695036	0.842040
O	O51	0.088571	0.169691	0.629284
O	O52	0.143460	0.509973	0.470802
O	O53	0.360507	0.258065	0.837047
O	O54	0.243614	0.028761	0.181843
O	O55	0.746455	0.503122	0.958511
O	O56	0.803112	0.842083	0.803242
O	O57	0.028409	0.588266	0.174251
O	O58	0.912716	0.360747	0.517730
O	O59	0.415245	0.835755	0.295716
O	O60	0.473184	0.176082	0.136502
O	O61	0.904126	0.704022	0.447026
O	O62	0.685413	0.607259	0.093224
O	O63	0.163034	0.573684	0.314146
O	O64	0.493493	0.853639	0.473043
O	O65	0.577399	0.050506	0.761556
O	O66	0.353554	0.945047	0.427675
O	O67	0.818711	0.904092	0.647455
O	O68	0.161269	0.192040	0.807713
O	O69	0.246283	0.382378	0.105789
O	O70	0.015371	0.273346	0.756321
O	O71	0.487589	0.241584	0.980938
O	O72	0.831853	0.522165	0.135247
O	O73	0.266798	0.709439	0.436599
O	O74	0.381538	0.585677	0.095946
O	O75	0.414609	0.096337	0.313103
O	O76	0.125744	0.146731	0.471379

O	O77	0.933450	0.040383	0.767220
O	O78	0.049672	0.918415	0.420887
O	O79	0.084937	0.432601	0.648253
O	O80	0.792515	0.483017	0.802400
O	O81	0.603261	0.374391	0.101465
O	O82	0.711289	0.254631	0.758205
O	O83	0.736508	0.756255	0.978088
O	O84	0.461039	0.814707	0.139719
O	O85	0.282609	0.079488	0.435000
O	O86	0.398963	0.303074	0.096523
O	O87	0.879686	0.810612	0.309131
O	O88	0.832873	0.479054	0.465773
O	O89	0.945070	0.406915	0.765899
O	O90	0.061304	0.627718	0.423743
O	O91	0.554498	0.170442	0.647671
O	O92	0.500189	0.825526	0.810453
O	O93	0.614711	0.739931	0.106840
O	O94	0.729069	0.968663	0.760414
O	O95	0.228541	0.494620	0.982484
O	O96	0.168112	0.152356	0.135864
O	O97	0.803407	0.662208	0.609101
Al	Al98	0.923958	0.599718	0.405612
Al	Al99	0.590359	0.934065	0.741030
Al	Al100	0.260587	0.268721	0.075544
Al	Al101	0.381814	0.836992	0.407812
Al	Al102	0.049394	0.168284	0.740143
Al	Al103	0.718110	0.502345	0.072429
Al	Al104	0.148574	0.054500	0.406008
Al	Al105	0.816632	0.392809	0.737894
Al	Al106	0.486263	0.724153	0.076792
Al	Al107	0.051694	0.396948	0.535857
Al	Al108	0.709814	0.727013	0.865874
Al	Al109	0.381298	0.062084	0.200895
Al	Al110	0.587909	0.161516	0.536695
Al	Al111	0.256698	0.496059	0.869384
Al	Al112	0.923303	0.826091	0.201667
Al	Al113	0.823186	0.942122	0.533733
Al	Al114	0.488022	0.271602	0.868403
Al	Al115	0.157617	0.605731	0.202144
Si	Si116	0.919921	0.823098	0.411056
P	P117	0.052244	0.169578	0.532546
P	P118	0.713883	0.501867	0.861220
P	P119	0.383245	0.835562	0.198075
P	P120	0.818165	0.386983	0.528862

P	P121	0.482057	0.724677	0.864586
P	P122	0.151330	0.057908	0.198202
P	P123	0.588902	0.930997	0.534337
P	P124	0.261431	0.271403	0.863869
P	P125	0.928370	0.602835	0.194735
P	P126	0.589384	0.164114	0.743325
P	P127	0.259831	0.494943	0.080208
P	P128	0.157713	0.605401	0.410878
P	P129	0.820971	0.939462	0.744331
P	P130	0.490506	0.273813	0.078771
P	P131	0.381403	0.065709	0.410561
P	P132	0.046402	0.395552	0.744083
P	P133	0.714078	0.728361	0.077173

TS-Methylation-MeOH-CO-Si-AlPO-34

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H	H2	0.645694	0.566157	0.670943
H	H3	0.684184	0.497490	0.582956
H	H4	0.630731	0.592308	0.551271
H	H5	0.819015	0.747378	0.620109
C	C6	0.648113	0.547706	0.601661
C	C7	0.498630	0.422382	0.604538
O	O8	0.076286	0.292086	0.502458
O	O9	0.297030	0.399565	0.839510
O	O10	0.816301	0.426819	0.618612
O	O11	0.483646	0.155256	0.462749
O	O12	0.726035	0.618355	0.827671

O	O13	0.963654	0.729621	0.168318
O	O14	0.490608	0.759734	0.956414
O	O15	0.145236	0.477303	0.801155
O	O16	0.401035	0.954982	0.165634
O	O17	0.611588	0.055591	0.521618
O	O18	0.158127	0.101095	0.287573
O	O19	0.821214	0.815740	0.122280
O	O20	0.713541	0.288274	0.498297
O	O21	0.596834	0.414659	0.836947
O	O22	0.561657	0.894221	0.623448
O	O23	0.846732	0.857680	0.467553
O	O24	0.374041	0.632511	0.832746
O	O25	0.266207	0.751342	0.176598
O	O26	0.239420	0.249400	0.955363
O	O27	0.516399	0.185058	0.800344
O	O28	0.044121	0.962548	0.168153
O	O29	0.933160	0.091344	0.517450
O	O30	0.898093	0.578474	0.285133
O	O31	0.186759	0.522964	0.130783
O	O32	0.699705	0.939977	0.500029
O	O33	0.577767	0.702619	0.835359
O	O34	0.095071	0.177706	0.623007
O	O35	0.146346	0.518068	0.464471
O	O36	0.365513	0.264910	0.829348
O	O37	0.248464	0.035701	0.176267
O	O38	0.749291	0.508570	0.951362
O	O39	0.807732	0.848486	0.795833
O	O40	0.032983	0.594951	0.166781
O	O41	0.918187	0.366192	0.514180
O	O42	0.420163	0.843792	0.288944
O	O43	0.477553	0.182373	0.129711
O	O44	0.903939	0.708381	0.440087
O	O45	0.689572	0.613623	0.085817
O	O46	0.165231	0.580448	0.307637
O	O47	0.498601	0.859270	0.466102
O	O48	0.580747	0.056908	0.749964
O	O49	0.361238	0.953328	0.422686
O	O50	0.820690	0.910501	0.640385
O	O51	0.165643	0.198282	0.801940
O	O52	0.250787	0.389162	0.098742
O	O53	0.020157	0.279733	0.750361
O	O54	0.492471	0.248595	0.974368
O	O55	0.836625	0.529007	0.128061
O	O56	0.270600	0.717204	0.429220

O	O57	0.386466	0.592424	0.088479
O	O58	0.420395	0.102650	0.306835
O	O59	0.129054	0.151082	0.465018
O	O60	0.938195	0.046681	0.759517
O	O61	0.054381	0.922331	0.415482
O	O62	0.091423	0.439132	0.642204
O	O63	0.797032	0.489951	0.794906
O	O64	0.608394	0.380544	0.094883
O	O65	0.716064	0.260880	0.753897
O	O66	0.742845	0.763090	0.971144
O	O67	0.465483	0.821387	0.133027
O	O68	0.286170	0.084507	0.427378
O	O69	0.404246	0.310285	0.089969
O	O70	0.885770	0.819469	0.302412
O	O71	0.839155	0.484873	0.460100
O	O72	0.950436	0.413789	0.758646
O	O73	0.065531	0.636862	0.417282
O	O74	0.561772	0.184847	0.641107
O	O75	0.504930	0.832869	0.803763
O	O76	0.619670	0.747088	0.098776
O	O77	0.733832	0.975993	0.755174
O	O78	0.233136	0.501373	0.975597
O	O79	0.173419	0.159400	0.129707
O	O80	0.814742	0.676806	0.606704
O	O81	0.411912	0.348017	0.612258
Al	Al82	0.927440	0.606205	0.398962
Al	Al83	0.595142	0.940373	0.733484
Al	Al84	0.265759	0.275757	0.069428
Al	Al85	0.387127	0.843797	0.401291
Al	Al86	0.054472	0.174894	0.733490
Al	Al87	0.722445	0.508824	0.065984
Al	Al88	0.151757	0.058884	0.399471
Al	Al89	0.821654	0.398489	0.731874
Al	Al90	0.490840	0.731083	0.070016
Al	Al91	0.058453	0.404109	0.529713
Al	Al92	0.714914	0.734276	0.859327
Al	Al93	0.386098	0.068745	0.194742
Al	Al94	0.591524	0.168978	0.530027
Al	Al95	0.261978	0.502966	0.862728
Al	Al96	0.928248	0.833035	0.194886
Al	Al97	0.827665	0.950471	0.526625
Al	Al98	0.492116	0.277122	0.862008
Al	Al99	0.162089	0.612541	0.195480
Si	Si100	0.923781	0.829401	0.404712

P	P101	0.057844	0.176690	0.526362
P	P102	0.717836	0.507727	0.854124
P	P103	0.387823	0.842546	0.191363
P	P104	0.823319	0.391910	0.522525
P	P105	0.486929	0.731997	0.857826
P	P106	0.155364	0.063941	0.191456
P	P107	0.593032	0.937221	0.527665
P	P108	0.266415	0.278054	0.857280
P	P109	0.933006	0.609304	0.187949
P	P110	0.594200	0.171764	0.736247
P	P111	0.264631	0.501870	0.073340
P	P112	0.161194	0.613350	0.404202
P	P113	0.825092	0.946223	0.737422
P	P114	0.495303	0.280459	0.072419
P	P115	0.386469	0.072876	0.404285
P	P116	0.051920	0.402070	0.737697
P	P117	0.718927	0.734987	0.070210

TS-Methylation-MeOH-NH3-Si-AlPO-34

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H	H3	0.669342	0.522039	0.573220
H	H4	0.658697	0.648493	0.551200
H	H5	0.840454	0.753721	0.624357
H	H6	0.460333	0.432398	0.641881
H	H7	0.457837	0.457148	0.535208
H	H8	0.453394	0.542054	0.609402

C	C9	0.662997	0.591626	0.597527
N	N10	0.487188	0.493495	0.595231
O	O11	0.075837	0.292056	0.502386
O	O12	0.296793	0.399799	0.839106
O	O13	0.817654	0.428772	0.618394
O	O14	0.483837	0.154091	0.462484
O	O15	0.728399	0.619885	0.829019
O	O16	0.964101	0.730074	0.167910
O	O17	0.490298	0.758270	0.956319
O	O18	0.145448	0.478150	0.801046
O	O19	0.401142	0.954909	0.166041
O	O20	0.612668	0.055876	0.520745
O	O21	0.158783	0.101733	0.287559
O	O22	0.821173	0.815963	0.122912
O	O23	0.713612	0.288457	0.499147
O	O24	0.597638	0.416178	0.838168
O	O25	0.561266	0.895120	0.624028
O	O26	0.846074	0.856453	0.467985
O	O27	0.374837	0.632005	0.831696
O	O28	0.266458	0.751274	0.177143
O	O29	0.240459	0.249802	0.955005
O	O30	0.517585	0.186022	0.800824
O	O31	0.044196	0.962873	0.168576
O	O32	0.933315	0.090898	0.516186
O	O33	0.899077	0.579765	0.285260
O	O34	0.186665	0.522888	0.130741
O	O35	0.699321	0.938462	0.501196
O	O36	0.578670	0.702841	0.835007
O	O37	0.093874	0.177337	0.623031
O	O38	0.147211	0.517884	0.464656
O	O39	0.366366	0.266127	0.828466
O	O40	0.248562	0.035819	0.176104
O	O41	0.750680	0.508927	0.951870
O	O42	0.808813	0.848601	0.795912
O	O43	0.033263	0.595248	0.166718
O	O44	0.918191	0.367032	0.513935
O	O45	0.421212	0.843521	0.288855
O	O46	0.477590	0.182292	0.129213
O	O47	0.905889	0.709266	0.440805
O	O48	0.689989	0.614009	0.085567
O	O49	0.165035	0.579871	0.307702
O	O50	0.498523	0.858867	0.466708
O	O51	0.582231	0.057386	0.752701
O	O52	0.360787	0.952590	0.421730

O	O53	0.823447	0.911652	0.640715
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O	O60	0.386497	0.592182	0.089118
O	O61	0.420451	0.102861	0.306578
O	O62	0.130102	0.152132	0.465242
O	O63	0.938677	0.047299	0.760732
O	O64	0.054247	0.923509	0.415990
O	O65	0.092001	0.439127	0.642122
O	O66	0.797812	0.490433	0.795467
O	O67	0.608423	0.380690	0.094788
O	O68	0.716691	0.261499	0.752980
O	O69	0.742900	0.764491	0.971685
O	O70	0.465400	0.821433	0.132507
O	O71	0.286344	0.084150	0.427301
O	O72	0.404298	0.310491	0.090522
O	O73	0.886082	0.818997	0.302696
O	O74	0.838821	0.484820	0.459266
O	O75	0.950581	0.414342	0.758123
O	O76	0.066002	0.636528	0.417807
O	O77	0.560690	0.181212	0.641586
O	O78	0.505283	0.832654	0.803966
O	O79	0.619567	0.746979	0.099484
O	O80	0.734167	0.975361	0.754933
O	O81	0.233891	0.502439	0.975535
O	O82	0.173466	0.159485	0.129512
O	O83	0.824830	0.679779	0.606935
Al	Al84	0.927979	0.606173	0.399098
Al	Al85	0.595623	0.940819	0.734180
Al	Al86	0.265985	0.275815	0.069219
Al	Al87	0.387619	0.843653	0.401095
Al	Al88	0.054575	0.175386	0.733800
Al	Al89	0.722739	0.508955	0.066064
Al	Al90	0.152423	0.059710	0.399530
Al	Al91	0.821666	0.399463	0.731301
Al	Al92	0.490835	0.730734	0.070148
Al	Al93	0.057855	0.404064	0.529698
Al	Al94	0.715812	0.734834	0.859888
Al	Al95	0.386287	0.068912	0.194539
Al	Al96	0.591672	0.169029	0.530325

Al	Al97	0.261980	0.503256	0.862656
Al	Al98	0.928518	0.833173	0.195041
Al	Al99	0.828023	0.950205	0.526841
Al	Al100	0.493029	0.278412	0.861612
Al	Al101	0.162156	0.612468	0.195595
Si	Si102	0.924133	0.829673	0.404947
P	P103	0.057718	0.176762	0.526120
P	P104	0.718921	0.508537	0.854660
P	P105	0.388169	0.842507	0.191456
P	P106	0.823089	0.392726	0.522643
P	P107	0.487426	0.731578	0.857620
P	P108	0.155648	0.064262	0.191454
P	P109	0.593152	0.937367	0.528031
P	P110	0.266984	0.278473	0.856870
P	P111	0.933422	0.609807	0.187931
P	P112	0.594765	0.171644	0.736797
P	P113	0.264692	0.501966	0.073365
P	P114	0.161586	0.612990	0.404307
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P	P116	0.495280	0.280678	0.072265
P	P117	0.386629	0.072518	0.403984
P	P118	0.052022	0.402571	0.737675
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TS-Methylation-MeOH-Toluene-Si-AlPO-34

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H	H4	0.686922	0.614852	0.528017
H	H5	0.862211	0.765851	0.634454
H	H6	0.514094	0.363643	0.400333
H	H7	0.484299	0.351284	0.562355
H	H8	0.479473	0.660333	0.556747
H	H9	0.509436	0.671621	0.394924
H	H10	0.556326	0.466266	0.264584
H	H11	0.612614	0.612330	0.274352
H	H12	0.470062	0.525758	0.251713
H	H13	0.464572	0.498480	0.641591
C	C14	0.665997	0.599810	0.597260
C	C15	0.491375	0.421891	0.525715
C	C16	0.489115	0.509668	0.572239
C	C17	0.488228	0.596324	0.522548
C	C18	0.504230	0.602043	0.431795
C	C19	0.516660	0.519846	0.386637
C	C20	0.540282	0.530908	0.289029
C	C21	0.507417	0.428659	0.434750
O	O22	0.073904	0.293569	0.499439
O	O23	0.296940	0.402205	0.836058
O	O24	0.145301	0.481055	0.798480
O	O25	0.162553	0.107183	0.284637
O	O26	0.090632	0.177496	0.619713
O	O27	0.365354	0.267274	0.826760
O	O28	0.247480	0.037111	0.172261
O	O29	0.476627	0.184995	0.126152
O	O30	0.165963	0.201235	0.797921
O	O31	0.249321	0.391003	0.095803
O	O32	0.020607	0.283749	0.747469
O	O33	0.419144	0.107332	0.303569
O	O34	0.130067	0.155041	0.462246
O	O35	0.093181	0.442850	0.639020
O	O36	0.285130	0.084935	0.425615
O	O37	0.402703	0.312604	0.087491
O	O38	0.172021	0.160597	0.125903
O	O39	0.730845	0.623790	0.828719
O	O40	0.963241	0.732394	0.164890
O	O41	0.821080	0.818938	0.119811
O	O42	0.559574	0.897470	0.621493
O	O43	0.844130	0.857121	0.465054
O	O44	0.897700	0.582336	0.282614
O	O45	0.698009	0.939240	0.499194
O	O46	0.578973	0.705431	0.830682

O	O47	0.808875	0.851921	0.793025
O	O48	0.908164	0.712566	0.438914
O	O49	0.690894	0.617271	0.081210
O	O50	0.497770	0.860417	0.463928
O	O51	0.825111	0.916772	0.638344
O	O52	0.835894	0.531222	0.126156
O	O53	0.880913	0.816433	0.300102
O	O54	0.838513	0.486561	0.455349
O	O55	0.505486	0.835760	0.802188
O	O56	0.618802	0.748345	0.098314
O	O57	0.733369	0.978046	0.752036
O	O58	0.815979	0.431559	0.615059
O	O59	0.483413	0.156109	0.459369
O	O60	0.612123	0.057747	0.517205
O	O61	0.713284	0.290543	0.495817
O	O62	0.597112	0.420384	0.835187
O	O63	0.518918	0.190547	0.797811
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O	O65	0.917958	0.369906	0.512257
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O	O72	0.560213	0.183404	0.638357
O	O73	0.490204	0.758126	0.953424
O	O74	0.749956	0.508350	0.949298
O	O75	0.741132	0.769083	0.968789
O	O76	0.401755	0.957754	0.164881
O	O77	0.374994	0.634668	0.827646
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O	O79	0.043022	0.965279	0.169096
O	O80	0.185605	0.525493	0.126575
O	O81	0.146821	0.519409	0.460843
O	O82	0.032647	0.597807	0.164599
O	O83	0.421447	0.843617	0.285695
O	O84	0.166684	0.582300	0.304035
O	O85	0.361169	0.954972	0.416843
O	O86	0.271351	0.718558	0.425971
O	O87	0.386289	0.594142	0.088693
O	O88	0.052031	0.926858	0.410060
O	O89	0.465003	0.824055	0.128600
O	O90	0.066223	0.638310	0.413294

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O	O92	0.493444	0.254041	0.971373
O	O93	0.236643	0.506176	0.972355
O	O94	0.847851	0.692231	0.617931
Al	Al95	0.264141	0.277455	0.065823
Al	Al96	0.054036	0.178353	0.730685
Al	Al97	0.152103	0.062805	0.396452
Al	Al98	0.057832	0.406551	0.526900
Al	Al99	0.385449	0.071423	0.191533
Al	Al100	0.493321	0.282357	0.858483
Al	Al101	0.928079	0.608826	0.396479
Al	Al102	0.594888	0.943525	0.731719
Al	Al103	0.490472	0.732422	0.067382
Al	Al104	0.715982	0.737885	0.856778
Al	Al105	0.927092	0.834820	0.193175
Al	Al106	0.827392	0.951527	0.523994
Al	Al107	0.722502	0.511087	0.062974
Al	Al108	0.821753	0.402470	0.727783
Al	Al109	0.591600	0.171152	0.527230
Al	Al110	0.387250	0.845437	0.397725
Al	Al111	0.262551	0.505903	0.858946
Al	Al112	0.161821	0.614995	0.192284
Si	Si113	0.922263	0.830547	0.402053
P	P114	0.056247	0.178374	0.522554
P	P115	0.155564	0.066789	0.188988
P	P116	0.266331	0.280726	0.853707
P	P117	0.264612	0.504405	0.070591
P	P118	0.385837	0.074793	0.400886
P	P119	0.052483	0.406078	0.734374
P	P120	0.718932	0.511040	0.852200
P	P121	0.592328	0.939262	0.525438
P	P122	0.932604	0.612226	0.185433
P	P123	0.826227	0.950367	0.735440
P	P124	0.718854	0.738538	0.067457
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P	P127	0.494591	0.283872	0.069574
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TS-Methylation-MeOH-TMB-Si-AlPO-34

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H	H6	0.521474	0.406431	0.260942
H	H7	0.585020	0.360652	0.339226
H	H8	0.659535	0.496323	0.294492
H	H9	0.453835	0.441638	0.691145
H	H10	0.474000	0.339682	0.637016
H	H11	0.346875	0.338004	0.625829
H	H12	0.398131	0.660097	0.582758
H	H13	0.462573	0.618972	0.663930
H	H14	0.328060	0.523801	0.626961
H	H15	0.637380	0.668919	0.280656
H	H16	0.523455	0.691234	0.292719
H	H17	0.506871	0.570733	0.237337
H	H18	0.525774	0.354394	0.485341
H	H19	0.465545	0.671252	0.438630
C	C20	0.658107	0.581032	0.582868
C	C21	0.577732	0.431835	0.317877
C	C22	0.514179	0.425176	0.474831
C	C23	0.479573	0.464544	0.548449
C	C24	0.437238	0.392935	0.630545
C	C25	0.456433	0.552793	0.533199
C	C26	0.409110	0.591549	0.605152
C	C27	0.479310	0.602037	0.449762
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C	C29	0.547583	0.627491	0.292873

C	C30	0.536504	0.474611	0.391825
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O	O59	0.496668	0.867435	0.465122
O	O60	0.821978	0.915661	0.640709
O	O61	0.835121	0.533161	0.128970
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O	O63	0.840021	0.489240	0.457942
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O	O76	0.935203	0.050865	0.761724
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O	O81	0.559977	0.180599	0.639236
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O	O83	0.754540	0.517756	0.950492
O	O84	0.743951	0.766507	0.970156
O	O85	0.400398	0.958928	0.165347
O	O86	0.371329	0.635453	0.835458
O	O87	0.265873	0.754991	0.174854
O	O88	0.042673	0.967619	0.170370
O	O89	0.186662	0.526327	0.131421
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O	O94	0.351543	0.952908	0.420076
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O	O96	0.385728	0.598145	0.085556
O	O97	0.055818	0.926712	0.410449
O	O98	0.466233	0.826049	0.133753
O	O99	0.067225	0.641592	0.417129
O	O100	0.233937	0.253011	0.955647
O	O101	0.488908	0.245246	0.973614
O	O102	0.228890	0.501235	0.976046
O	O103	0.831494	0.687884	0.615504
Al	Al104	0.265207	0.279817	0.068846
Al	Al105	0.051489	0.178231	0.733801
Al	Al106	0.151980	0.064399	0.398797
Al	Al107	0.055452	0.406496	0.529247
Al	Al108	0.384646	0.072376	0.194143
Al	Al109	0.489979	0.279944	0.861983
Al	Al110	0.929193	0.611376	0.398909
Al	Al111	0.592627	0.944243	0.733271
Al	Al112	0.490489	0.736899	0.068131
Al	Al113	0.712794	0.736950	0.858522
Al	Al114	0.927332	0.836758	0.194777
Al	Al115	0.826254	0.952252	0.526627
Al	Al116	0.722873	0.513361	0.064053
Al	Al117	0.819205	0.402450	0.730084

Al	Al118	0.593260	0.171197	0.528356
Al	Al119	0.383527	0.847541	0.400646
Al	Al120	0.258857	0.505264	0.863113
Al	Al121	0.161517	0.616421	0.194818
Si	Si122	0.924944	0.833174	0.403660
P	P123	0.053528	0.178537	0.526285
P	P124	0.155153	0.068771	0.191400
P	P125	0.263318	0.281063	0.857700
P	P126	0.264069	0.505529	0.073168
P	P127	0.383341	0.074913	0.403786
P	P128	0.049708	0.406243	0.737015
P	P129	0.716501	0.512027	0.854213
P	P130	0.593496	0.942023	0.526165
P	P131	0.932959	0.614085	0.187423
P	P132	0.823291	0.949916	0.737685
P	P133	0.718396	0.738539	0.068896
P	P134	0.821768	0.396374	0.521205
P	P135	0.592853	0.174246	0.735533
P	P136	0.494579	0.282580	0.070309
P	P137	0.387075	0.846403	0.190837
P	P138	0.484528	0.735972	0.857839
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TS-Methylation-ZCH3-C2-Si-AlPO-34

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H	H4	0.610492	0.474621	0.642833
H	H5	0.625221	0.613666	0.656501
H	H6	0.510100	0.449598	0.501123
H	H7	0.524798	0.588994	0.514115
C	C8	0.732016	0.615433	0.508368
C	C9	0.597970	0.540011	0.615976
C	C10	0.542948	0.526303	0.538706
O	O11	0.081894	0.293310	0.500770
O	O12	0.298272	0.399019	0.843288
O	O13	0.822988	0.434126	0.616962
O	O14	0.486501	0.155113	0.461398
O	O15	0.732400	0.620964	0.828362
O	O16	0.966533	0.730399	0.166480
O	O17	0.494720	0.761210	0.955611
O	O18	0.148345	0.478641	0.800885
O	O19	0.404547	0.955418	0.165688
O	O20	0.617033	0.057878	0.516706
O	O21	0.157673	0.094788	0.288968
O	O22	0.823227	0.815982	0.122481
O	O23	0.714912	0.291468	0.500047
O	O24	0.600634	0.417468	0.839728
O	O25	0.566377	0.900344	0.623516
O	O26	0.848795	0.860437	0.465112
O	O27	0.377326	0.632033	0.833312
O	O28	0.269798	0.751817	0.176590
O	O29	0.239563	0.245440	0.956058
O	O30	0.522088	0.189146	0.799619
O	O31	0.047162	0.963143	0.165190
O	O32	0.935284	0.093571	0.515720
O	O33	0.904416	0.581135	0.284273
O	O34	0.190350	0.522658	0.132734
O	O35	0.702108	0.938807	0.499538
O	O36	0.581446	0.703199	0.834853
O	O37	0.095915	0.177417	0.622594
O	O38	0.142189	0.518631	0.464307
O	O39	0.368301	0.265705	0.830812
O	O40	0.251280	0.035757	0.175272
O	O41	0.756384	0.510410	0.950938
O	O42	0.811635	0.849618	0.795249
O	O43	0.036693	0.596413	0.164033
O	O44	0.917862	0.359699	0.518184
O	O45	0.424057	0.843791	0.288648
O	O46	0.480858	0.183217	0.129714
O	O47	0.896033	0.702827	0.438214

O	O48	0.693209	0.614121	0.084503
O	O49	0.164457	0.581641	0.307785
O	O50	0.501494	0.859015	0.466972
O	O51	0.585008	0.058317	0.754481
O	O52	0.364471	0.952691	0.421908
O	O53	0.824343	0.915469	0.640481
O	O54	0.168882	0.198937	0.801455
O	O55	0.254164	0.389775	0.097003
O	O56	0.023401	0.280888	0.750598
O	O57	0.495397	0.247910	0.973843
O	O58	0.839062	0.528956	0.128537
O	O59	0.275880	0.715861	0.429179
O	O60	0.389236	0.593129	0.087574
O	O61	0.421667	0.102218	0.306322
O	O62	0.129867	0.147749	0.465159
O	O63	0.941397	0.048356	0.761125
O	O64	0.056748	0.917065	0.418855
O	O65	0.095974	0.439467	0.641686
O	O66	0.799464	0.490507	0.793361
O	O67	0.611607	0.381140	0.093569
O	O68	0.720087	0.262212	0.749189
O	O69	0.745952	0.764779	0.970822
O	O70	0.468940	0.821928	0.132494
O	O71	0.288024	0.082177	0.428043
O	O72	0.407404	0.310655	0.089008
O	O73	0.891676	0.821721	0.301624
O	O74	0.849323	0.483370	0.456058
O	O75	0.953994	0.415438	0.756738
O	O76	0.073086	0.647947	0.417332
O	O77	0.561555	0.178243	0.640594
O	O78	0.507063	0.831868	0.802156
O	O79	0.621892	0.746280	0.098613
O	O80	0.736764	0.976652	0.757350
O	O81	0.234031	0.503480	0.976104
O	O82	0.177638	0.162071	0.133344
Al	Al83	0.932927	0.607884	0.397920
Al	Al84	0.598879	0.942098	0.734618
Al	Al85	0.268505	0.275532	0.069404
Al	Al86	0.391090	0.843727	0.401056
Al	Al87	0.057425	0.175772	0.733611
Al	Al88	0.726079	0.509242	0.064809
Al	Al89	0.153058	0.054762	0.401184
Al	Al90	0.825242	0.400358	0.729849
Al	Al91	0.493858	0.731598	0.068998

Al	Al92	0.060234	0.402711	0.529851
Al	Al93	0.718938	0.735705	0.858694
Al	Al94	0.388981	0.069033	0.194040
Al	Al95	0.593978	0.169305	0.529324
Al	Al96	0.264187	0.503370	0.863451
Al	Al97	0.931745	0.834104	0.193271
Al	Al98	0.831183	0.952620	0.527266
Al	Al99	0.495786	0.279330	0.861692
Al	Al100	0.164955	0.613324	0.195028
Si	Si101	0.925524	0.829557	0.404718
P	P102	0.060417	0.176858	0.525630
P	P103	0.722285	0.509541	0.854240
P	P104	0.391511	0.842988	0.191122
P	P105	0.827383	0.392231	0.522748
P	P106	0.490279	0.732093	0.857154
P	P107	0.157955	0.063351	0.191645
P	P108	0.597010	0.939335	0.526881
P	P109	0.268422	0.277399	0.858434
P	P110	0.936894	0.610491	0.186420
P	P111	0.597516	0.171964	0.735876
P	P112	0.267264	0.502533	0.073126
P	P113	0.163403	0.616094	0.404296
P	P114	0.828592	0.947999	0.737934
P	P115	0.498430	0.280692	0.071545
P	P116	0.388918	0.072074	0.403868
P	P117	0.055499	0.403141	0.737180
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TS-Methylation-ZCH3-C3-Si-AlPO-34

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H	H4	0.616275	0.477240	0.634508
H	H5	0.624127	0.612592	0.653561
H	H6	0.503538	0.445605	0.502595
H	H7	0.400803	0.552805	0.507653
H	H8	0.518180	0.624663	0.440099
H	H9	0.520842	0.671413	0.550620
C	C10	0.740736	0.619964	0.511256
C	C11	0.599022	0.540869	0.611009
C	C12	0.531840	0.522400	0.539919
C	C13	0.492101	0.598105	0.508651
O	O14	0.083646	0.294244	0.501213
O	O15	0.298224	0.398903	0.842898
O	O16	0.824475	0.434379	0.616883
O	O17	0.486897	0.155350	0.461129
O	O18	0.732570	0.620842	0.828422
O	O19	0.966980	0.730309	0.165566
O	O20	0.494073	0.761663	0.955558
O	O21	0.148232	0.478331	0.801021
O	O22	0.404430	0.955280	0.165227
O	O23	0.617958	0.058851	0.516801
O	O24	0.157599	0.095184	0.288709
O	O25	0.823148	0.815735	0.122403
O	O26	0.715344	0.291906	0.500138
O	O27	0.600845	0.417386	0.840863
O	O28	0.566047	0.900326	0.623028
O	O29	0.851103	0.863473	0.464064
O	O30	0.377045	0.631984	0.833422
O	O31	0.269792	0.751600	0.176141
O	O32	0.240184	0.245976	0.956071
O	O33	0.522188	0.189090	0.799638
O	O34	0.047199	0.963086	0.165181
O	O35	0.935115	0.095226	0.516426
O	O36	0.904887	0.582689	0.284686
O	O37	0.190366	0.522388	0.132907
O	O38	0.702154	0.938948	0.499328
O	O39	0.581184	0.703091	0.835491
O	O40	0.096456	0.177193	0.622667
O	O41	0.143472	0.518969	0.464603
O	O42	0.368303	0.265594	0.830518

O	O43	0.251346	0.035704	0.175459
O	O44	0.757770	0.511008	0.950897
O	O45	0.811228	0.849370	0.794840
O	O46	0.036467	0.595703	0.164719
O	O47	0.918336	0.359621	0.517339
O	O48	0.423399	0.843930	0.288645
O	O49	0.481187	0.183296	0.129816
O	O50	0.896225	0.703421	0.439399
O	O51	0.693304	0.613892	0.084354
O	O52	0.165412	0.582218	0.308083
O	O53	0.501908	0.860332	0.466340
O	O54	0.584856	0.058148	0.754245
O	O55	0.363645	0.952943	0.422110
O	O56	0.824633	0.915536	0.640005
O	O57	0.168676	0.198581	0.801778
O	O58	0.254598	0.389805	0.097444
O	O59	0.023522	0.280693	0.750280
O	O60	0.494147	0.246765	0.973744
O	O61	0.838775	0.528508	0.129268
O	O62	0.276459	0.716199	0.429705
O	O63	0.389287	0.593248	0.087626
O	O64	0.422039	0.102087	0.306118
O	O65	0.128724	0.146793	0.464988
O	O66	0.941251	0.048161	0.760889
O	O67	0.058017	0.916683	0.417842
O	O68	0.095702	0.439743	0.641815
O	O69	0.799286	0.490213	0.793146
O	O70	0.611890	0.380833	0.092562
O	O71	0.720037	0.261995	0.748835
O	O72	0.746367	0.764624	0.970558
O	O73	0.469254	0.821873	0.132889
O	O74	0.288732	0.083775	0.427584
O	O75	0.407728	0.310725	0.089338
O	O76	0.892042	0.820451	0.301331
O	O77	0.849923	0.483622	0.455970
O	O78	0.953754	0.414885	0.757218
O	O79	0.073402	0.647758	0.417723
O	O80	0.561248	0.178089	0.640512
O	O81	0.506944	0.831578	0.801690
O	O82	0.621888	0.746052	0.098070
O	O83	0.736656	0.976541	0.756656
O	O84	0.234027	0.502914	0.976264
O	O85	0.177725	0.161842	0.132894
Al	Al86	0.933294	0.608344	0.398345

Al	Al87	0.598728	0.941975	0.734266
Al	Al88	0.268928	0.275657	0.069419
Al	Al89	0.390885	0.844500	0.401027
Al	Al90	0.057526	0.175509	0.733624
Al	Al91	0.726493	0.509180	0.064600
Al	Al92	0.153318	0.054950	0.400816
Al	Al93	0.825243	0.400183	0.729812
Al	Al94	0.493878	0.731710	0.068815
Al	Al95	0.060565	0.402881	0.529931
Al	Al96	0.718786	0.735361	0.858392
Al	Al97	0.389125	0.068999	0.193866
Al	Al98	0.594267	0.169958	0.529324
Al	Al99	0.264152	0.503132	0.863525
Al	Al100	0.931950	0.833750	0.192799
Al	Al101	0.831690	0.953802	0.527077
Al	Al102	0.495729	0.279224	0.861633
Al	Al103	0.165116	0.613177	0.195165
Si	Si104	0.926398	0.830341	0.404377
P	P105	0.060652	0.177172	0.525893
P	P106	0.722578	0.509534	0.854352
P	P107	0.391390	0.842941	0.190937
P	P108	0.828021	0.392425	0.522594
P	P109	0.490025	0.732085	0.857198
P	P110	0.158020	0.063379	0.191491
P	P111	0.597335	0.940130	0.526569
P	P112	0.268582	0.277397	0.858314
P	P113	0.936987	0.610530	0.186593
P	P114	0.597401	0.171858	0.735730
P	P115	0.267393	0.502367	0.073303
P	P116	0.164054	0.616358	0.404632
P	P117	0.828493	0.947808	0.737512
P	P118	0.498419	0.280415	0.071323
P	P119	0.389124	0.072645	0.403695
P	P120	0.055349	0.402926	0.737321
P	P121	0.721739	0.735091	0.069207

TS-Methylation-ZCH3-MeOH-Si-AlPO-34

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H	H4	0.808683	0.728816	0.563455
H	H5	0.511098	0.572262	0.670181
H	H6	0.536309	0.578271	0.553690
H	H7	0.610514	0.701067	0.619437
C	C8	0.573731	0.610695	0.618200
C	C9	0.780979	0.645039	0.542386
O	O10	0.086225	0.296532	0.502851
O	O11	0.299583	0.399823	0.842897
O	O12	0.829666	0.436488	0.617813
O	O13	0.489595	0.155866	0.460645
O	O14	0.728169	0.619573	0.821688
O	O15	0.967832	0.732051	0.164196
O	O16	0.489197	0.763077	0.956076
O	O17	0.148755	0.478290	0.801901
O	O18	0.404958	0.956810	0.164583
O	O19	0.621396	0.060622	0.516891
O	O20	0.160786	0.098274	0.289304
O	O21	0.823643	0.818078	0.124748
O	O22	0.716996	0.293276	0.502344
O	O23	0.600921	0.416827	0.844100
O	O24	0.568879	0.902396	0.623452
O	O25	0.857572	0.868687	0.464865
O	O26	0.378846	0.632079	0.832146
O	O27	0.270941	0.753135	0.177236
O	O28	0.240158	0.247360	0.956697
O	O29	0.522196	0.189104	0.799654
O	O30	0.047945	0.965345	0.166952
O	O31	0.935123	0.098634	0.517298
O	O32	0.904155	0.586129	0.284927
O	O33	0.191435	0.524741	0.132320
O	O34	0.702588	0.938243	0.498562

O	O35	0.582851	0.705533	0.841120
O	O36	0.096370	0.176832	0.623362
O	O37	0.144021	0.520937	0.465630
O	O38	0.368289	0.265496	0.831495
O	O39	0.252223	0.037439	0.174895
O	O40	0.759829	0.521622	0.950722
O	O41	0.811455	0.848081	0.793390
O	O42	0.037101	0.597217	0.166655
O	O43	0.919812	0.360260	0.516046
O	O44	0.424718	0.847552	0.289416
O	O45	0.482694	0.186093	0.131592
O	O46	0.901587	0.707064	0.444016
O	O47	0.693272	0.615547	0.088692
O	O48	0.166740	0.582199	0.308419
O	O49	0.502127	0.861972	0.467437
O	O50	0.586669	0.059016	0.756464
O	O51	0.363052	0.953684	0.423433
O	O52	0.825815	0.917196	0.639682
O	O53	0.168982	0.199399	0.802458
O	O54	0.255819	0.391843	0.097864
O	O55	0.023508	0.280860	0.750645
O	O56	0.492936	0.244104	0.974233
O	O57	0.839939	0.530074	0.129007
O	O58	0.276575	0.717776	0.429515
O	O59	0.391062	0.595177	0.088851
O	O60	0.421739	0.101740	0.306560
O	O61	0.127778	0.146962	0.465386
O	O62	0.942294	0.047805	0.761919
O	O63	0.062666	0.918865	0.417079
O	O64	0.094086	0.440770	0.643062
O	O65	0.799120	0.490581	0.794319
O	O66	0.613387	0.382113	0.089538
O	O67	0.719990	0.262959	0.748774
O	O68	0.753897	0.762678	0.971208
O	O69	0.470695	0.823698	0.134295
O	O70	0.291478	0.087330	0.429197
O	O71	0.409177	0.312765	0.088419
O	O72	0.894716	0.818926	0.302923
O	O73	0.851007	0.485005	0.456863
O	O74	0.953645	0.414817	0.760446
O	O75	0.073604	0.648359	0.416232
O	O76	0.560738	0.175387	0.640902
O	O77	0.508077	0.831915	0.801225
O	O78	0.624416	0.750534	0.092954

O	O79	0.737763	0.976554	0.757824
O	O80	0.237103	0.505645	0.976363
O	O81	0.178662	0.163808	0.133377
O	O82	0.658205	0.579097	0.630985
Al	Al83	0.933362	0.609533	0.398738
Al	Al84	0.600187	0.943177	0.734685
Al	Al85	0.269985	0.277565	0.069945
Al	Al86	0.391284	0.845988	0.401863
Al	Al87	0.057911	0.175937	0.734167
Al	Al88	0.727366	0.512147	0.065376
Al	Al89	0.156260	0.057821	0.401417
Al	Al90	0.825933	0.400670	0.730633
Al	Al91	0.494174	0.733896	0.069001
Al	Al92	0.062017	0.404604	0.530611
Al	Al93	0.720509	0.736623	0.859829
Al	Al94	0.389816	0.070416	0.194253
Al	Al95	0.595938	0.170749	0.529719
Al	Al96	0.265420	0.503976	0.863608
Al	Al97	0.933466	0.835260	0.194017
Al	Al98	0.833260	0.956604	0.526384
Al	Al99	0.495127	0.277950	0.862421
Al	Al100	0.166172	0.614608	0.195969
Si	Si101	0.930773	0.832771	0.405651
P	P102	0.061241	0.178705	0.526639
P	P103	0.721973	0.510679	0.854232
P	P104	0.392426	0.845040	0.191706
P	P105	0.830074	0.393616	0.523068
P	P106	0.489844	0.733367	0.858394
P	P107	0.159462	0.065608	0.192153
P	P108	0.598873	0.941235	0.526602
P	P109	0.268948	0.278091	0.858930
P	P110	0.937570	0.612544	0.186888
P	P111	0.597657	0.171757	0.736125
P	P112	0.269157	0.504606	0.073729
P	P113	0.164686	0.617334	0.404609
P	P114	0.829539	0.948264	0.737536
P	P115	0.499119	0.281228	0.071085
P	P116	0.390287	0.073843	0.404510
P	P117	0.055091	0.403208	0.738599
P	P118	0.724158	0.736802	0.070087

TS-Methylation-ZCH3-C4-iso-Si-AlPO-34

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H	H3	0.724574	0.689066	0.463296
H	H4	0.402954	0.559805	0.385738
H	H5	0.537365	0.620473	0.340691
H	H6	0.515958	0.670338	0.443407
H	H7	0.497490	0.350406	0.435571
H	H8	0.502298	0.418140	0.333607
H	H9	0.380471	0.357724	0.397786
H	H10	0.558280	0.463050	0.568213
H	H11	0.569326	0.601418	0.571129
C	C12	0.728811	0.614363	0.471728
C	C13	0.553950	0.528882	0.532854
C	C14	0.508053	0.510607	0.450187
C	C15	0.491054	0.596137	0.403428
C	C16	0.471695	0.403408	0.402087
O	O17	0.086579	0.293686	0.504885
O	O18	0.302179	0.400190	0.848070
O	O19	0.828425	0.435190	0.621247
O	O20	0.490551	0.152610	0.466064
O	O21	0.736598	0.621720	0.831825
O	O22	0.969509	0.731292	0.171556
O	O23	0.498812	0.762202	0.959968
O	O24	0.151731	0.478939	0.805018
O	O25	0.409201	0.956612	0.172295
O	O26	0.626827	0.060813	0.519138
O	O27	0.164405	0.097964	0.293429
O	O28	0.827727	0.817913	0.124564
O	O29	0.718174	0.293668	0.504215

O	O30	0.604562	0.418384	0.844713
O	O31	0.569863	0.904111	0.628172
O	O32	0.858280	0.865326	0.469446
O	O33	0.379756	0.633423	0.838234
O	O34	0.274162	0.752912	0.180823
O	O35	0.242987	0.246456	0.960561
O	O36	0.525262	0.190392	0.802965
O	O37	0.051149	0.964631	0.171068
O	O38	0.937210	0.095001	0.521024
O	O39	0.908100	0.581018	0.288439
O	O40	0.193838	0.523229	0.137286
O	O41	0.704371	0.934502	0.504873
O	O42	0.583655	0.703022	0.838699
O	O43	0.098854	0.176916	0.626997
O	O44	0.144867	0.518262	0.468054
O	O45	0.371794	0.266442	0.835588
O	O46	0.255216	0.036572	0.179057
O	O47	0.759892	0.512565	0.955592
O	O48	0.815147	0.851070	0.801241
O	O49	0.041111	0.598450	0.168276
O	O50	0.920752	0.358603	0.521898
O	O51	0.428319	0.842196	0.293244
O	O52	0.484831	0.183963	0.133904
O	O53	0.897728	0.702844	0.438928
O	O54	0.697095	0.614861	0.091358
O	O55	0.169147	0.582566	0.311907
O	O56	0.505267	0.861751	0.471720
O	O57	0.589419	0.059429	0.761930
O	O58	0.365435	0.951696	0.423444
O	O59	0.829981	0.916868	0.645944
O	O60	0.172720	0.200260	0.805846
O	O61	0.258670	0.391042	0.102047
O	O62	0.026763	0.281347	0.754478
O	O63	0.499221	0.249192	0.978133
O	O64	0.843140	0.529775	0.132667
O	O65	0.280653	0.715311	0.434003
O	O66	0.392873	0.594491	0.092499
O	O67	0.424932	0.105164	0.310861
O	O68	0.130446	0.144955	0.469498
O	O69	0.945270	0.049449	0.767003
O	O70	0.062815	0.915313	0.418133
O	O71	0.098931	0.439878	0.645731
O	O72	0.803891	0.490811	0.799103
O	O73	0.615367	0.382082	0.098408

O	O74	0.723495	0.263246	0.753017
O	O75	0.745788	0.761711	0.974657
O	O76	0.473349	0.823558	0.136506
O	O77	0.292475	0.083914	0.433770
O	O78	0.411221	0.311437	0.093941
O	O79	0.892090	0.823150	0.304709
O	O80	0.855223	0.484770	0.460447
O	O81	0.957337	0.415781	0.761287
O	O82	0.078400	0.650098	0.421067
O	O83	0.564989	0.174883	0.644671
O	O84	0.510473	0.832728	0.806539
O	O85	0.625331	0.746674	0.104225
O	O86	0.740674	0.977731	0.761455
O	O87	0.237737	0.503964	0.980745
O	O88	0.181496	0.163081	0.137562
Al	Al89	0.937931	0.608375	0.401854
Al	Al90	0.602796	0.943442	0.739730
Al	Al91	0.272442	0.276596	0.073636
Al	Al92	0.394586	0.844035	0.405284
Al	Al93	0.060945	0.176326	0.738201
Al	Al94	0.729841	0.510245	0.069185
Al	Al95	0.157324	0.054801	0.405078
Al	Al96	0.828804	0.401476	0.734200
Al	Al97	0.497889	0.732761	0.073155
Al	Al98	0.063238	0.402274	0.534074
Al	Al99	0.720964	0.734878	0.861733
Al	Al100	0.392944	0.070270	0.198615
Al	Al101	0.599499	0.169472	0.533569
Al	Al102	0.267525	0.504137	0.867800
Al	Al103	0.934712	0.835415	0.196816
Al	Al104	0.835357	0.952817	0.532944
Al	Al105	0.499676	0.280586	0.865635
Al	Al106	0.169033	0.614539	0.199167
Si	Si107	0.930418	0.831763	0.406724
P	P108	0.062855	0.176467	0.530245
P	P109	0.726111	0.510575	0.858449
P	P110	0.395942	0.843638	0.195913
P	P111	0.831605	0.393141	0.527178
P	P112	0.493424	0.732772	0.861377
P	P113	0.162501	0.064877	0.196154
P	P114	0.601949	0.940764	0.531366
P	P115	0.272182	0.278535	0.862904
P	P116	0.940647	0.611422	0.190651
P	P117	0.601200	0.172188	0.740564

P	P118	0.271079	0.503452	0.077705
P	P119	0.167684	0.616585	0.408540
P	P120	0.832698	0.948993	0.743280
P	P121	0.502328	0.281602	0.075851
P	P122	0.392222	0.072285	0.408115
P	P123	0.058703	0.403577	0.741363
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TS-Methylation-ZCH3-TME-Si-AlPO-34

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H	H3	0.720946	0.688216	0.461039
H	H4	0.411744	0.565687	0.389218
H	H5	0.541278	0.613749	0.337495
H	H6	0.531961	0.679534	0.435020
H	H7	0.522615	0.364049	0.424425
H	H8	0.493308	0.424650	0.332601
H	H9	0.390756	0.351724	0.413666
H	H10	0.603705	0.464877	0.647661
H	H11	0.547276	0.371122	0.557175
H	H12	0.459059	0.387657	0.631869
H	H13	0.493703	0.592237	0.650586
H	H14	0.558270	0.689413	0.564101
H	H15	0.638135	0.656349	0.636475
C	C16	0.724879	0.612898	0.464251
C	C17	0.538945	0.432055	0.596683
C	C18	0.559390	0.622224	0.600127

C	C19	0.541999	0.525500	0.543260
C	C20	0.515217	0.514945	0.454474
C	C21	0.500833	0.599596	0.402376
C	C22	0.480254	0.408498	0.403807
O	O23	0.086332	0.293296	0.504257
O	O24	0.302063	0.400230	0.847744
O	O25	0.829520	0.435743	0.621194
O	O26	0.489673	0.153105	0.466838
O	O27	0.736592	0.621646	0.830604
O	O28	0.969263	0.731296	0.171801
O	O29	0.498152	0.762358	0.959781
O	O30	0.152512	0.479653	0.804249
O	O31	0.409945	0.957021	0.172963
O	O32	0.626244	0.060582	0.516345
O	O33	0.162711	0.095509	0.293489
O	O34	0.827737	0.818108	0.124464
O	O35	0.717525	0.293409	0.505187
O	O36	0.605140	0.418610	0.845844
O	O37	0.570193	0.906989	0.628410
O	O38	0.857280	0.865237	0.469132
O	O39	0.380453	0.633096	0.837628
O	O40	0.274522	0.753322	0.181050
O	O41	0.244016	0.246818	0.960539
O	O42	0.525627	0.191191	0.802490
O	O43	0.051617	0.964507	0.169397
O	O44	0.936861	0.094956	0.522091
O	O45	0.908345	0.580412	0.288072
O	O46	0.194377	0.523777	0.137363
O	O47	0.703862	0.934188	0.505371
O	O48	0.584226	0.703153	0.839403
O	O49	0.099855	0.177889	0.626856
O	O50	0.144020	0.518403	0.467999
O	O51	0.372695	0.267505	0.835053
O	O52	0.255623	0.036563	0.179071
O	O53	0.761507	0.514812	0.955515
O	O54	0.815647	0.851235	0.801387
O	O55	0.041516	0.599108	0.167475
O	O56	0.920257	0.358115	0.521263
O	O57	0.428561	0.841957	0.293622
O	O58	0.485223	0.184361	0.134354
O	O59	0.893693	0.700937	0.437575
O	O60	0.696910	0.614775	0.091999
O	O61	0.167524	0.583042	0.311998
O	O62	0.504361	0.860231	0.472626

O	O63	0.590391	0.059898	0.764442
O	O64	0.366434	0.952094	0.423794
O	O65	0.829812	0.916212	0.646006
O	O66	0.173280	0.200050	0.805855
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O	O68	0.027643	0.281516	0.755000
O	O69	0.498270	0.247890	0.978187
O	O70	0.843419	0.529871	0.132311
O	O71	0.279363	0.715629	0.434069
O	O72	0.393189	0.594580	0.092135
O	O73	0.424812	0.105500	0.311362
O	O74	0.129241	0.143543	0.469414
O	O75	0.945860	0.049445	0.766535
O	O76	0.061568	0.913442	0.419103
O	O77	0.098618	0.438943	0.645263
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O	O79	0.615970	0.381926	0.097215
O	O80	0.723685	0.263506	0.752316
O	O81	0.746725	0.760909	0.974583
O	O82	0.473609	0.823695	0.136714
O	O83	0.291311	0.082480	0.434004
O	O84	0.411874	0.311979	0.093902
O	O85	0.892563	0.824735	0.304220
O	O86	0.853968	0.483960	0.460142
O	O87	0.957687	0.415541	0.761283
O	O88	0.076920	0.650036	0.421873
O	O89	0.564450	0.171782	0.644862
O	O90	0.510935	0.832376	0.805969
O	O91	0.625614	0.747143	0.103308
O	O92	0.741254	0.977896	0.761472
O	O93	0.237823	0.504454	0.980596
O	O94	0.182378	0.163611	0.138166
Al	Al95	0.936385	0.607667	0.401680
Al	Al96	0.603468	0.944200	0.740199
Al	Al97	0.272980	0.276902	0.073834
Al	Al98	0.394389	0.843634	0.405593
Al	Al99	0.061604	0.176446	0.738105
Al	Al100	0.730166	0.510666	0.069064
Al	Al101	0.156070	0.053027	0.405286
Al	Al102	0.829369	0.401648	0.734030
Al	Al103	0.497920	0.732999	0.073026
Al	Al104	0.062783	0.401815	0.533478
Al	Al105	0.721614	0.734915	0.861780
Al	Al106	0.393367	0.070581	0.199066

Al	Al107	0.598933	0.168739	0.533414
Al	Al108	0.267644	0.504351	0.867725
Al	Al109	0.935005	0.835899	0.196401
Al	Al110	0.834983	0.952673	0.533137
Al	Al111	0.500010	0.280693	0.865942
Al	Al112	0.169132	0.614968	0.199115
Si	Si113	0.929024	0.831214	0.406500
P	P114	0.062698	0.176267	0.530217
P	P115	0.726773	0.511089	0.858486
P	P116	0.396352	0.843826	0.196299
P	P117	0.831322	0.392909	0.527160
P	P118	0.493751	0.732776	0.861340
P	P119	0.162570	0.064435	0.195930
P	P120	0.601570	0.941037	0.531094
P	P121	0.272690	0.278756	0.862825
P	P122	0.940840	0.611469	0.190371
P	P123	0.601479	0.171852	0.740903
P	P124	0.271287	0.503757	0.077578
P	P125	0.166408	0.616816	0.408733
P	P126	0.833128	0.948976	0.743210
P	P127	0.502493	0.281482	0.075769
P	P128	0.391941	0.072285	0.408540
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TS-Methylation-ZCH3-CO-Si-AlPO-34

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H	H3	0.770472	0.712997	0.532148
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C	C5	0.643732	0.573783	0.621331
O	O6	0.079384	0.291866	0.499174
O	O7	0.296194	0.397499	0.841942
O	O8	0.823204	0.433982	0.615858
O	O9	0.484331	0.151793	0.459644
O	O10	0.730579	0.619790	0.826881
O	O11	0.964493	0.729259	0.163183
O	O12	0.491394	0.760352	0.954121
O	O13	0.146581	0.477187	0.798910
O	O14	0.401582	0.953906	0.164132
O	O15	0.618054	0.058259	0.514138
O	O16	0.156017	0.094014	0.287592
O	O17	0.819958	0.814429	0.122602
O	O18	0.712119	0.291312	0.499671
O	O19	0.598854	0.416254	0.839117
O	O20	0.564081	0.900975	0.621870
O	O21	0.847994	0.859719	0.463970
O	O22	0.375539	0.630553	0.831622
O	O23	0.267143	0.750259	0.175122
O	O24	0.236507	0.243600	0.954511
O	O25	0.519876	0.187945	0.797827
O	O26	0.044028	0.962085	0.164628
O	O27	0.932319	0.092540	0.514281
O	O28	0.902202	0.582502	0.282942
O	O29	0.187532	0.521217	0.130681
O	O30	0.699236	0.935832	0.498211
O	O31	0.579700	0.702078	0.835037
O	O32	0.093005	0.175710	0.621022
O	O33	0.138948	0.517123	0.462883
O	O34	0.366012	0.264088	0.829736
O	O35	0.248216	0.033998	0.173351
O	O36	0.755186	0.509856	0.949748
O	O37	0.809548	0.847445	0.793299
O	O38	0.033877	0.594598	0.163216
O	O39	0.914951	0.357444	0.515824
O	O40	0.421783	0.842345	0.286855
O	O41	0.478083	0.181826	0.128291
O	O42	0.896247	0.702488	0.440524
O	O43	0.690891	0.612872	0.082973
O	O44	0.161875	0.579524	0.306135
O	O45	0.499216	0.859329	0.465377

O	O46	0.583892	0.057186	0.755084
O	O47	0.360143	0.949996	0.419400
O	O48	0.822957	0.913048	0.638534
O	O49	0.166784	0.197513	0.799718
O	O50	0.251605	0.388440	0.095229
O	O51	0.020933	0.279181	0.749327
O	O52	0.493093	0.245935	0.972236
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O	O54	0.273704	0.713953	0.427349
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O	O56	0.418382	0.100603	0.304691
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O	O58	0.939387	0.046328	0.759350
O	O59	0.055642	0.916287	0.417308
O	O60	0.092104	0.437461	0.640154
O	O61	0.797480	0.489509	0.791807
O	O62	0.609012	0.379645	0.091657
O	O63	0.717728	0.261008	0.747257
O	O64	0.745834	0.764404	0.969854
O	O65	0.466298	0.820795	0.130639
O	O66	0.286081	0.081236	0.427263
O	O67	0.404800	0.309154	0.086830
O	O68	0.890374	0.816933	0.300866
O	O69	0.847531	0.482654	0.454993
O	O70	0.951699	0.413811	0.756503
O	O71	0.071195	0.647082	0.415165
O	O72	0.558699	0.173902	0.639214
O	O73	0.505315	0.830228	0.800260
O	O74	0.619318	0.744987	0.096161
O	O75	0.734858	0.974583	0.754898
O	O76	0.231804	0.502254	0.974243
O	O77	0.174903	0.160713	0.131848
O	O78	0.558417	0.542555	0.651912
Al	Al79	0.931009	0.606591	0.396404
Al	Al80	0.596939	0.940900	0.733137
Al	Al81	0.265845	0.274107	0.067776
Al	Al82	0.388518	0.842093	0.399191
Al	Al83	0.055179	0.174256	0.732134
Al	Al84	0.723592	0.507828	0.063583
Al	Al85	0.151694	0.054282	0.399776
Al	Al86	0.823232	0.398851	0.728781
Al	Al87	0.491086	0.730318	0.067320
Al	Al88	0.057521	0.401018	0.528187
Al	Al89	0.717165	0.734563	0.857952

Al	Al90	0.386046	0.067543	0.192455
Al	Al91	0.591994	0.167684	0.527757
Al	Al92	0.262310	0.501994	0.861690
Al	Al93	0.929490	0.832238	0.191940
Al	Al94	0.828864	0.951676	0.525571
Al	Al95	0.493634	0.277911	0.860177
Al	Al96	0.162510	0.611708	0.193497
Si	Si97	0.924684	0.828678	0.403775
P	P98	0.057685	0.175464	0.524110
P	P99	0.720448	0.508314	0.853174
P	P100	0.388885	0.841598	0.189482
P	P101	0.825389	0.391063	0.521487
P	P102	0.488113	0.730799	0.855886
P	P103	0.155418	0.062182	0.190272
P	P104	0.595178	0.938774	0.525072
P	P105	0.266097	0.275839	0.856999
P	P106	0.934507	0.609606	0.184753
P	P107	0.595271	0.169999	0.734655
P	P108	0.264745	0.501200	0.071331
P	P109	0.161153	0.614485	0.402520
P	P110	0.826706	0.945949	0.736004
P	P111	0.495819	0.279088	0.069800
P	P112	0.386143	0.070058	0.402251
P	P113	0.052978	0.401440	0.735908
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TS-Methylation-ZCH3-H2O-Si-AlPO-34

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H	H4	0.816447	0.732163	0.569275
H	H5	0.618042	0.620025	0.630980
C	C6	0.781363	0.647053	0.548642
O	O7	0.083934	0.294746	0.502376
O	O8	0.298337	0.399004	0.842224
O	O9	0.827283	0.434294	0.617431
O	O10	0.488071	0.155000	0.460788
O	O11	0.727968	0.618758	0.820888
O	O12	0.966961	0.729699	0.163745
O	O13	0.494195	0.762190	0.955759
O	O14	0.148137	0.478117	0.801079
O	O15	0.404119	0.955199	0.164219
O	O16	0.619245	0.058736	0.517273
O	O17	0.157986	0.097141	0.288027
O	O18	0.823704	0.815955	0.122864
O	O19	0.716379	0.291172	0.501277
O	O20	0.600606	0.415900	0.844057
O	O21	0.565497	0.899479	0.622898
O	O22	0.855239	0.866380	0.463792
O	O23	0.377306	0.631798	0.833715
O	O24	0.269432	0.751497	0.175543
O	O25	0.241160	0.246853	0.955902
O	O26	0.521331	0.187920	0.799164
O	O27	0.047701	0.963123	0.165406
O	O28	0.934354	0.096309	0.517296
O	O29	0.902642	0.583694	0.284442
O	O30	0.190793	0.522788	0.132555
O	O31	0.701470	0.937267	0.499373
O	O32	0.581491	0.703508	0.836086
O	O33	0.096018	0.176212	0.622896
O	O34	0.144700	0.519899	0.465046
O	O35	0.367788	0.265386	0.829492
O	O36	0.251881	0.036147	0.176010
O	O37	0.760023	0.521481	0.950175
O	O38	0.811024	0.847689	0.794035
O	O39	0.035897	0.594581	0.166488
O	O40	0.919685	0.361296	0.514815
O	O41	0.422466	0.844450	0.288521
O	O42	0.481817	0.183859	0.129947
O	O43	0.901610	0.706638	0.442908
O	O44	0.692196	0.613073	0.088667

O	O45	0.167188	0.582106	0.308139
O	O46	0.501400	0.860831	0.466028
O	O47	0.585421	0.057668	0.755180
O	O48	0.362765	0.953200	0.422120
O	O49	0.825049	0.914068	0.639337
O	O50	0.167787	0.198305	0.802303
O	O51	0.255109	0.390041	0.097534
O	O52	0.023134	0.280362	0.750262
O	O53	0.490502	0.242566	0.973063
O	O54	0.839080	0.527731	0.128438
O	O55	0.274669	0.717720	0.429818
O	O56	0.389823	0.593358	0.087195
O	O57	0.423694	0.102059	0.305767
O	O58	0.127483	0.146625	0.464833
O	O59	0.940865	0.047107	0.760699
O	O60	0.061180	0.918775	0.416690
O	O61	0.093095	0.439917	0.642364
O	O62	0.798435	0.489630	0.793514
O	O63	0.613041	0.379733	0.087923
O	O64	0.719359	0.261542	0.749272
O	O65	0.747870	0.759191	0.970987
O	O66	0.469225	0.821807	0.133214
O	O67	0.290611	0.086488	0.426424
O	O68	0.409040	0.311775	0.088728
O	O69	0.894084	0.818205	0.301780
O	O70	0.847725	0.484134	0.456938
O	O71	0.952891	0.413990	0.759857
O	O72	0.071182	0.644817	0.416138
O	O73	0.560967	0.175995	0.640481
O	O74	0.506805	0.831357	0.801703
O	O75	0.623114	0.747672	0.096337
O	O76	0.736140	0.974608	0.755966
O	O77	0.234300	0.502686	0.976160
O	O78	0.178193	0.161497	0.131588
O	O79	0.664616	0.586636	0.637634
Al	Al80	0.931542	0.608051	0.398294
Al	Al81	0.598332	0.941345	0.733796
Al	Al82	0.269857	0.276224	0.069309
Al	Al83	0.390081	0.844792	0.401035
Al	Al84	0.057137	0.175182	0.733566
Al	Al85	0.726757	0.510206	0.064915
Al	Al86	0.155063	0.057320	0.400162
Al	Al87	0.824956	0.399075	0.730185
Al	Al88	0.493967	0.731993	0.069115

Al	Al89	0.061388	0.403889	0.529874
Al	Al90	0.718643	0.735320	0.859114
Al	Al91	0.389692	0.069214	0.193864
Al	Al92	0.594788	0.169536	0.529233
Al	Al93	0.264021	0.502872	0.863458
Al	Al94	0.933013	0.833392	0.193010
Al	Al95	0.831951	0.954426	0.526059
Al	Al96	0.493930	0.276934	0.861335
Al	Al97	0.165376	0.612991	0.195580
Si	Si98	0.929581	0.831490	0.404720
P	P99	0.060321	0.177421	0.526224
P	P100	0.721633	0.509583	0.853897
P	P101	0.390913	0.843000	0.190745
P	P102	0.828546	0.392578	0.522325
P	P103	0.489779	0.732266	0.857590
P	P104	0.158500	0.063899	0.191300
P	P105	0.597008	0.939384	0.526377
P	P106	0.268432	0.277489	0.857982
P	P107	0.936494	0.610166	0.186546
P	P108	0.596988	0.170803	0.735661
P	P109	0.267793	0.502499	0.073251
P	P110	0.163842	0.616155	0.404433
P	P111	0.828461	0.946780	0.736818
P	P112	0.498162	0.279460	0.070104
P	P113	0.390032	0.073385	0.403337
P	P114	0.054483	0.402602	0.737948
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TS-Methylation-ZCH3-NH3-Si-AlPO-34

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H	H3	0.802436	0.588880	0.559407
H	H4	0.810563	0.726246	0.563510
H	H5	0.596290	0.620772	0.616218
H	H6	0.666567	0.590880	0.688252
C	C7	0.781699	0.647394	0.531632
N	N8	0.639758	0.580271	0.624398
O	O9	0.086043	0.295324	0.501353
O	O10	0.299777	0.399128	0.845206
O	O11	0.828138	0.434939	0.618473
O	O12	0.489748	0.153524	0.461733
O	O13	0.733800	0.621036	0.831178
O	O14	0.968103	0.730410	0.164103
O	O15	0.494321	0.761435	0.957083
O	O16	0.150462	0.478819	0.801648
O	O17	0.403635	0.954777	0.165502
O	O18	0.623324	0.060550	0.519490
O	O19	0.160028	0.097706	0.290041
O	O20	0.823017	0.816018	0.126671
O	O21	0.716838	0.293056	0.501913
O	O22	0.603047	0.417493	0.842115
O	O23	0.568013	0.900520	0.624484
O	O24	0.860020	0.870918	0.463924
O	O25	0.379801	0.632082	0.833892
O	O26	0.269807	0.751190	0.178435
O	O27	0.240618	0.244426	0.956855
O	O28	0.523480	0.188792	0.801034
O	O29	0.047516	0.963634	0.168188
O	O30	0.934951	0.098080	0.519471
O	O31	0.906263	0.587520	0.287030
O	O32	0.190715	0.522567	0.133669
O	O33	0.702756	0.936803	0.500142
O	O34	0.583966	0.703922	0.838489
O	O35	0.097928	0.178841	0.623817
O	O36	0.143235	0.520290	0.466875
O	O37	0.370274	0.266390	0.831723
O	O38	0.251848	0.036510	0.176405
O	O39	0.759110	0.510690	0.953348
O	O40	0.813187	0.848418	0.795132
O	O41	0.036119	0.594611	0.167550
O	O42	0.919349	0.358384	0.517888

O	O43	0.424931	0.845658	0.289583
O	O44	0.481619	0.183324	0.130857
O	O45	0.901798	0.706787	0.446649
O	O46	0.694794	0.614959	0.085060
O	O47	0.165393	0.580895	0.309692
O	O48	0.503082	0.863008	0.467797
O	O49	0.587888	0.058909	0.756109
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O	O51	0.826944	0.914978	0.640457
O	O52	0.170874	0.199228	0.802096
O	O53	0.254062	0.389537	0.096870
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O	O57	0.277953	0.716416	0.430094
O	O58	0.389888	0.592909	0.089144
O	O59	0.423003	0.101683	0.306956
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O	O61	0.943484	0.047479	0.761607
O	O62	0.064428	0.917367	0.416885
O	O63	0.095192	0.438175	0.643265
O	O64	0.801759	0.491548	0.795147
O	O65	0.611757	0.381474	0.094675
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O	O69	0.292416	0.087354	0.429251
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O	O71	0.895318	0.815659	0.303721
O	O72	0.852968	0.484531	0.457712
O	O73	0.955322	0.415149	0.760055
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O	O75	0.562754	0.177492	0.641942
O	O76	0.509738	0.832113	0.803260
O	O77	0.622658	0.746569	0.098745
O	O78	0.738950	0.976055	0.757354
O	O79	0.235514	0.505252	0.976916
O	O80	0.177220	0.161816	0.133699
Al	Al81	0.935119	0.609667	0.400670
Al	Al82	0.601034	0.942380	0.735482
Al	Al83	0.268848	0.275352	0.070144
Al	Al84	0.391825	0.845091	0.402013
Al	Al85	0.058984	0.175885	0.734806
Al	Al86	0.727004	0.509307	0.067123

Al	Al87	0.156812	0.057034	0.401888
Al	Al88	0.827299	0.400911	0.731614
Al	Al89	0.494111	0.731488	0.070361
Al	Al90	0.061929	0.402985	0.530989
Al	Al91	0.721699	0.737049	0.861520
Al	Al92	0.389435	0.068969	0.194849
Al	Al93	0.596797	0.170000	0.530784
Al	Al94	0.266104	0.503886	0.864493
Al	Al95	0.933537	0.833200	0.194604
Al	Al96	0.833644	0.955667	0.527769
Al	Al97	0.497297	0.279214	0.862924
Al	Al98	0.165371	0.612562	0.196996
Si	Si99	0.932276	0.833135	0.406071
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P	P101	0.724524	0.509511	0.856824
P	P102	0.391481	0.843034	0.192131
P	P103	0.830168	0.392517	0.523925
P	P104	0.492046	0.732448	0.858837
P	P105	0.158797	0.064381	0.193039
P	P106	0.599347	0.940455	0.528042
P	P107	0.270047	0.277431	0.859481
P	P108	0.937568	0.611250	0.188414
P	P109	0.599158	0.172053	0.737186
P	P110	0.267860	0.502812	0.073986
P	P111	0.165126	0.616967	0.405844
P	P112	0.830688	0.947323	0.738051
P	P113	0.498811	0.280675	0.072756
P	P114	0.390691	0.072806	0.404701
P	P115	0.056417	0.402651	0.739114
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TS-Methylation-ZCH3-Toluene-Si-AlPO-34

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H	H2	0.768377	0.572118	0.541338
H	H3	0.767284	0.705100	0.529269
H	H4	0.412452	0.447900	0.291301
H	H5	0.327194	0.495816	0.337770
H	H6	0.295311	0.356388	0.354899
H	H7	0.548756	0.377017	0.579710
H	H8	0.458138	0.643477	0.435285
H	H9	0.424872	0.318457	0.449552
H	H10	0.621778	0.567396	0.642767
H	H11	0.579970	0.702030	0.566500
C	C12	0.743500	0.623200	0.505472
C	C13	0.530759	0.435846	0.546924
C	C14	0.579122	0.546199	0.579312
C	C15	0.547957	0.619044	0.539752
C	C16	0.478886	0.585639	0.466016
C	C17	0.434961	0.477684	0.431260
C	C18	0.362918	0.442569	0.349797
C	C19	0.460919	0.402989	0.473852
O	O20	0.091769	0.296902	0.493631
O	O21	0.304801	0.401301	0.835436
O	O22	0.828587	0.434328	0.608958
O	O23	0.493267	0.156025	0.453820
O	O24	0.737688	0.622611	0.819991
O	O25	0.973095	0.733249	0.159280
O	O26	0.499430	0.763332	0.948442
O	O27	0.153821	0.480292	0.794708
O	O28	0.410347	0.957536	0.158866
O	O29	0.624154	0.059963	0.510483
O	O30	0.166576	0.100110	0.282232
O	O31	0.829557	0.818131	0.114736
O	O32	0.722797	0.292312	0.491010
O	O33	0.606441	0.419162	0.832629
O	O34	0.573563	0.901184	0.615893
O	O35	0.860604	0.866963	0.458922
O	O36	0.382855	0.634471	0.825909
O	O37	0.276187	0.753775	0.168949
O	O38	0.245593	0.248731	0.949041
O	O39	0.527850	0.191124	0.791572

O	O40	0.052357	0.966053	0.160783
O	O41	0.941296	0.098425	0.508512
O	O42	0.909760	0.584092	0.277240
O	O43	0.195966	0.524515	0.125266
O	O44	0.708237	0.940207	0.490926
O	O45	0.587100	0.705973	0.828070
O	O46	0.101677	0.178679	0.615655
O	O47	0.148199	0.520700	0.456684
O	O48	0.373608	0.266810	0.823843
O	O49	0.256600	0.037443	0.168085
O	O50	0.762487	0.513418	0.943243
O	O51	0.817244	0.851641	0.787331
O	O52	0.042580	0.598700	0.157736
O	O53	0.925223	0.360198	0.511923
O	O54	0.430020	0.845481	0.281419
O	O55	0.486630	0.185244	0.122350
O	O56	0.902824	0.704923	0.432950
O	O57	0.698898	0.616132	0.077414
O	O58	0.172276	0.583679	0.300280
O	O59	0.507498	0.861937	0.459517
O	O60	0.590168	0.060181	0.745286
O	O61	0.368759	0.954097	0.413932
O	O62	0.830176	0.919546	0.633042
O	O63	0.174377	0.201020	0.794719
O	O64	0.261392	0.392442	0.091595
O	O65	0.029212	0.283139	0.742920
O	O66	0.500894	0.249626	0.966362
O	O67	0.845296	0.531814	0.121193
O	O68	0.282657	0.717555	0.421956
O	O69	0.395564	0.595965	0.081825
O	O70	0.427052	0.104601	0.298960
O	O71	0.134842	0.147869	0.458255
O	O72	0.947040	0.050760	0.754537
O	O73	0.064873	0.917428	0.408044
O	O74	0.103997	0.442586	0.634831
O	O75	0.805363	0.492223	0.785986
O	O76	0.617903	0.383097	0.085798
O	O77	0.726324	0.263996	0.742255
O	O78	0.752289	0.766106	0.962899
O	O79	0.475719	0.824886	0.125310
O	O80	0.295214	0.086071	0.421619
O	O81	0.413707	0.313026	0.081969
O	O82	0.895269	0.820868	0.295013
O	O83	0.858261	0.484448	0.448397

O	O84	0.960384	0.418184	0.748596
O	O85	0.079957	0.650730	0.408492
O	O86	0.568993	0.182519	0.632478
O	O87	0.512501	0.834367	0.794950
O	O88	0.628404	0.749036	0.090518
O	O89	0.742388	0.979053	0.750886
O	O90	0.241660	0.504960	0.969269
O	O91	0.183558	0.164178	0.125955
Al	Al92	0.938830	0.609744	0.390978
Al	Al93	0.604647	0.944040	0.727137
Al	Al94	0.274782	0.277964	0.062291
Al	Al95	0.396825	0.846144	0.393639
Al	Al96	0.063184	0.177908	0.726657
Al	Al97	0.732246	0.511612	0.057125
Al	Al98	0.159448	0.056152	0.393735
Al	Al99	0.831088	0.402341	0.722194
Al	Al100	0.500139	0.734227	0.061662
Al	Al101	0.068036	0.405102	0.523152
Al	Al102	0.724457	0.737339	0.850511
Al	Al103	0.394557	0.071136	0.186604
Al	Al104	0.601471	0.171682	0.521582
Al	Al105	0.270600	0.505416	0.856172
Al	Al106	0.936942	0.835833	0.186788
Al	Al107	0.838331	0.956755	0.519755
Al	Al108	0.501612	0.281203	0.854009
Al	Al109	0.171009	0.615486	0.187619
Si	Si110	0.932432	0.831327	0.397542
P	P111	0.066994	0.179293	0.518686
P	P112	0.728001	0.511556	0.846386
P	P113	0.397723	0.845163	0.183824
P	P114	0.834773	0.392944	0.515042
P	P115	0.495738	0.734511	0.849917
P	P116	0.164156	0.066190	0.185087
P	P117	0.603718	0.941298	0.519410
P	P118	0.274392	0.279663	0.851182
P	P119	0.942789	0.613166	0.179465
P	P120	0.603727	0.174514	0.727900
P	P121	0.273955	0.504776	0.066586
P	P122	0.169849	0.618255	0.396636
P	P123	0.834269	0.950621	0.730865
P	P124	0.504528	0.282771	0.064007
P	P125	0.394936	0.074110	0.396518
P	P126	0.061906	0.405647	0.729984
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TS-Methylation-ZCH3-TMB-Si-AlPO-34

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H	H4	0.404309	0.337667	0.279174
H	H5	0.526042	0.335471	0.310986
H	H6	0.535371	0.445304	0.245131
H	H7	0.628927	0.524609	0.669701
H	H8	0.609026	0.402859	0.615531
H	H9	0.494863	0.407119	0.662692
H	H10	0.482934	0.690439	0.610880
H	H11	0.601077	0.685506	0.648887
H	H12	0.467441	0.576185	0.674331
H	H13	0.482087	0.580473	0.244205
H	H14	0.407360	0.628338	0.308234
H	H15	0.345496	0.486195	0.278030
H	H16	0.561521	0.370778	0.462405
H	H17	0.449778	0.656322	0.459123
C	C18	0.732179	0.619648	0.492686
C	C19	0.490970	0.389427	0.300308
C	C20	0.537591	0.434083	0.461272
C	C21	0.551012	0.495692	0.539933
C	C22	0.573249	0.456082	0.626611
C	C23	0.515697	0.576116	0.539011
C	C24	0.516709	0.635584	0.622300
C	C25	0.475867	0.594748	0.459911

C	C26	0.466741	0.535956	0.382030
C	C27	0.423143	0.559626	0.298887
C	C28	0.498496	0.453676	0.382643
O	O29	0.086820	0.296314	0.500847
O	O30	0.302776	0.404730	0.842601
O	O31	0.834048	0.440082	0.617474
O	O32	0.492179	0.155595	0.461008
O	O33	0.736086	0.624591	0.829784
O	O34	0.968849	0.734669	0.166636
O	O35	0.501001	0.775728	0.956516
O	O36	0.154163	0.485067	0.798855
O	O37	0.407986	0.959059	0.164733
O	O38	0.633034	0.066833	0.507748
O	O39	0.165716	0.102648	0.289516
O	O40	0.823802	0.818676	0.126243
O	O41	0.718221	0.298922	0.502254
O	O42	0.606824	0.421720	0.849874
O	O43	0.571967	0.917653	0.624261
O	O44	0.861998	0.870425	0.468189
O	O45	0.380643	0.637757	0.839858
O	O46	0.273706	0.755666	0.178269
O	O47	0.240262	0.250802	0.955560
O	O48	0.525347	0.197179	0.794589
O	O49	0.049074	0.968420	0.168758
O	O50	0.935232	0.098809	0.519185
O	O51	0.912690	0.589068	0.286840
O	O52	0.194780	0.526965	0.133900
O	O53	0.702851	0.933562	0.502301
O	O54	0.584336	0.706707	0.841609
O	O55	0.098453	0.179672	0.623250
O	O56	0.145188	0.520959	0.464198
O	O57	0.374024	0.272507	0.833645
O	O58	0.253166	0.037777	0.174942
O	O59	0.769074	0.521881	0.953576
O	O60	0.814522	0.854375	0.799031
O	O61	0.040355	0.601671	0.163589
O	O62	0.920282	0.358523	0.516464
O	O63	0.427254	0.850798	0.290644
O	O64	0.483551	0.188259	0.132876
O	O65	0.901956	0.708162	0.441880
O	O66	0.695330	0.615950	0.088625
O	O67	0.166174	0.585218	0.308263
O	O68	0.504309	0.866079	0.469273
O	O69	0.590833	0.064235	0.764575

O	O70	0.361701	0.953748	0.424768
O	O71	0.829545	0.919445	0.643644
O	O72	0.175442	0.204292	0.799874
O	O73	0.260645	0.395401	0.098633
O	O74	0.029098	0.285706	0.751899
O	O75	0.496472	0.242139	0.973849
O	O76	0.840705	0.531464	0.133519
O	O77	0.282204	0.717174	0.429408
O	O78	0.390984	0.598734	0.080532
O	O79	0.422381	0.101456	0.307284
O	O80	0.127076	0.145575	0.465693
O	O81	0.946016	0.052769	0.764238
O	O82	0.065481	0.919119	0.414100
O	O83	0.096636	0.442114	0.641297
O	O84	0.802972	0.493607	0.795419
O	O85	0.615419	0.382977	0.088683
O	O86	0.723823	0.267385	0.747090
O	O87	0.750954	0.766020	0.973640
O	O88	0.473237	0.825017	0.136273
O	O89	0.294259	0.090864	0.430326
O	O90	0.411548	0.314227	0.084198
O	O91	0.892993	0.822826	0.304011
O	O92	0.857917	0.487547	0.456247
O	O93	0.957816	0.418564	0.759571
O	O94	0.080407	0.654996	0.420168
O	O95	0.565540	0.169976	0.639454
O	O96	0.511172	0.833776	0.799054
O	O97	0.622767	0.747143	0.098640
O	O98	0.741579	0.982151	0.758746
O	O99	0.229213	0.500133	0.976193
O	O100	0.182303	0.166344	0.133177
Al	Al101	0.939972	0.614201	0.400675
Al	Al102	0.604240	0.949424	0.736809
Al	Al103	0.272097	0.279788	0.068444
Al	Al104	0.393384	0.848612	0.403074
Al	Al105	0.061627	0.179633	0.734444
Al	Al106	0.730927	0.513239	0.066127
Al	Al107	0.158086	0.058853	0.401287
Al	Al108	0.830329	0.405613	0.730688
Al	Al109	0.497250	0.737810	0.068137
Al	Al110	0.063327	0.404556	0.529442
Al	Al111	0.722460	0.738789	0.861244
Al	Al112	0.390936	0.071408	0.194508
Al	Al113	0.601409	0.171503	0.527804

Al	Al114	0.266791	0.507412	0.864356
Al	Al115	0.933975	0.837920	0.195662
Al	Al116	0.835316	0.955745	0.530326
Al	Al117	0.500433	0.282904	0.863288
Al	Al118	0.167851	0.617323	0.195459
Si	Si119	0.932506	0.834569	0.406092
P	P120	0.061498	0.178855	0.526732
P	P121	0.728781	0.515033	0.857809
P	P122	0.395135	0.847427	0.192701
P	P123	0.833803	0.396208	0.523390
P	P124	0.494625	0.738551	0.859791
P	P125	0.161771	0.067969	0.192475
P	P126	0.603585	0.946346	0.526235
P	P127	0.272861	0.283155	0.858397
P	P128	0.940860	0.615555	0.188205
P	P129	0.601868	0.174935	0.736322
P	P130	0.269069	0.505667	0.072011
P	P131	0.167732	0.619595	0.405223
P	P132	0.833044	0.952534	0.740784
P	P133	0.501458	0.281833	0.069772
P	P134	0.391344	0.074547	0.405464
P	P135	0.059312	0.407279	0.737547
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TS-Ethylation-C3-C2H5Z-Si-AlPO-34

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H	H4	0.533105	0.602289	0.348672
H	H5	0.500993	0.664100	0.439333
H	H6	0.740278	0.696473	0.637346
H	H7	0.847526	0.672091	0.604469
H	H8	0.723689	0.559368	0.643437
H	H9	0.520092	0.465434	0.598555
H	H10	0.529290	0.602781	0.588424
H	H11	0.478598	0.429926	0.441463
C	C12	0.756790	0.636006	0.605329
C	C13	0.719678	0.615675	0.512272
C	C14	0.519589	0.528379	0.556284
C	C15	0.492964	0.508515	0.469361
C	C16	0.480869	0.585529	0.407692
O	O17	0.082957	0.291975	0.509538
O	O18	0.296450	0.396096	0.850549
O	O19	0.823315	0.427046	0.624856
O	O20	0.485180	0.152691	0.468377
O	O21	0.731270	0.618053	0.836926
O	O22	0.963864	0.727579	0.175634
O	O23	0.492044	0.757560	0.962954
O	O24	0.146478	0.475054	0.807843
O	O25	0.403047	0.952898	0.174024
O	O26	0.614575	0.054513	0.525165
O	O27	0.157455	0.093725	0.295728
O	O28	0.821655	0.813325	0.128336
O	O29	0.713976	0.287387	0.506413
O	O30	0.598276	0.414519	0.846942
O	O31	0.565668	0.896294	0.630838
O	O32	0.850368	0.860621	0.473255
O	O33	0.374493	0.629080	0.840440
O	O34	0.268272	0.749166	0.183927
O	O35	0.236752	0.242537	0.963206
O	O36	0.518772	0.185339	0.806790
O	O37	0.045096	0.960287	0.173271
O	O38	0.932419	0.093294	0.521096
O	O39	0.901370	0.576271	0.291755
O	O40	0.187969	0.519795	0.140023
O	O41	0.699203	0.935072	0.505046
O	O42	0.578431	0.699604	0.841915
O	O43	0.091308	0.170800	0.629711
O	O44	0.143408	0.516559	0.471572
O	O45	0.365739	0.262157	0.838355
O	O46	0.249304	0.032927	0.181818

O	O47	0.754476	0.505382	0.957876
O	O48	0.808123	0.845382	0.800213
O	O49	0.034811	0.594347	0.171606
O	O50	0.917743	0.358022	0.520462
O	O51	0.422612	0.840175	0.296105
O	O52	0.479003	0.180554	0.136639
O	O53	0.893738	0.700796	0.443774
O	O54	0.691726	0.611665	0.089757
O	O55	0.162993	0.579102	0.315078
O	O56	0.498237	0.856105	0.474805
O	O57	0.580561	0.053931	0.760782
O	O58	0.362337	0.950832	0.427932
O	O59	0.823209	0.917676	0.647400
O	O60	0.166791	0.196112	0.808395
O	O61	0.252216	0.387026	0.104794
O	O62	0.021562	0.277706	0.756539
O	O63	0.493840	0.245743	0.980978
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O	O67	0.419621	0.101297	0.313256
O	O68	0.126554	0.143809	0.472005
O	O69	0.938868	0.045487	0.770815
O	O70	0.055965	0.913785	0.422935
O	O71	0.090917	0.437407	0.649030
O	O72	0.796762	0.486790	0.799846
O	O73	0.609295	0.378856	0.101194
O	O74	0.717161	0.257511	0.758143
O	O75	0.743037	0.763324	0.977016
O	O76	0.467434	0.819577	0.139675
O	O77	0.286620	0.080831	0.435622
O	O78	0.405024	0.307631	0.096174
O	O79	0.886777	0.820153	0.308539
O	O80	0.845108	0.481360	0.465278
O	O81	0.951177	0.411028	0.767040
O	O82	0.069093	0.642072	0.425294
O	O83	0.560292	0.176567	0.647810
O	O84	0.504435	0.828750	0.809685
O	O85	0.619831	0.743012	0.106093
O	O86	0.734208	0.974302	0.766300
O	O87	0.232734	0.500800	0.983588
O	O88	0.175084	0.158805	0.139793
Al	Al89	0.929358	0.604289	0.405411
Al	Al90	0.596321	0.938713	0.742076

Al	Al91	0.266195	0.272670	0.076392
Al	Al92	0.388671	0.841697	0.408136
Al	Al93	0.054845	0.172005	0.740906
Al	Al94	0.724268	0.506245	0.071414
Al	Al95	0.151476	0.052279	0.407695
Al	Al96	0.822647	0.395309	0.738217
Al	Al97	0.491913	0.728743	0.076301
Al	Al98	0.059282	0.400652	0.536731
Al	Al99	0.716008	0.732207	0.864899
Al	Al100	0.387065	0.066643	0.201112
Al	Al101	0.592336	0.166723	0.536678
Al	Al102	0.262121	0.500180	0.870719
Al	Al103	0.928870	0.831561	0.200706
Al	Al104	0.829491	0.951831	0.533589
Al	Al105	0.493601	0.276470	0.868645
Al	Al106	0.162936	0.610801	0.202310
Si	Si107	0.923888	0.827697	0.410921
P	P108	0.057988	0.173879	0.532668
P	P109	0.720114	0.505892	0.861360
P	P110	0.389988	0.840248	0.198629
P	P111	0.826072	0.388505	0.529380
P	P112	0.487606	0.728746	0.864373
P	P113	0.156189	0.060763	0.198596
P	P114	0.594766	0.936014	0.534228
P	P115	0.266149	0.274368	0.865596
P	P116	0.934452	0.607464	0.194230
P	P117	0.594524	0.168395	0.743251
P	P118	0.265291	0.499776	0.080762
P	P119	0.161321	0.613113	0.411691
P	P120	0.826153	0.946227	0.745627
P	P121	0.496445	0.278167	0.078667
P	P122	0.387266	0.070555	0.410791
P	P123	0.052685	0.399861	0.744760
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TS-Ethylation-C4-iso-C2H5Z-Si-AlPO-34

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H	H3	0.391424	0.556170	0.391414
H	H4	0.526186	0.604199	0.350059
H	H5	0.506597	0.668869	0.444992
H	H6	0.465122	0.340438	0.472638
H	H7	0.500464	0.405650	0.366584
H	H8	0.365787	0.354916	0.408946
H	H9	0.749194	0.701473	0.634512
H	H10	0.852598	0.669467	0.605266
H	H11	0.724681	0.561847	0.642635
H	H12	0.523571	0.466892	0.596670
H	H13	0.539172	0.606832	0.585511
C	C14	0.762801	0.638324	0.603929
C	C15	0.725681	0.617605	0.510571
C	C16	0.523565	0.529964	0.554146
C	C17	0.487455	0.506419	0.468946
C	C18	0.478444	0.589639	0.411485
C	C19	0.453870	0.395730	0.427935
O	O20	0.084131	0.292084	0.509401
O	O21	0.296514	0.395784	0.851162
O	O22	0.823496	0.426384	0.624682
O	O23	0.484381	0.150402	0.468948
O	O24	0.731215	0.617764	0.836924
O	O25	0.963857	0.727622	0.175237
O	O26	0.491646	0.757228	0.962753
O	O27	0.146523	0.474599	0.807618
O	O28	0.403100	0.952855	0.174786
O	O29	0.615664	0.054839	0.525958
O	O30	0.157534	0.093273	0.296257
O	O31	0.821668	0.813434	0.128010
O	O32	0.713281	0.287411	0.506049
O	O33	0.598083	0.414229	0.846938
O	O34	0.565984	0.895859	0.630846
O	O35	0.851048	0.861483	0.472962

O	O36	0.374339	0.628795	0.840189
O	O37	0.268076	0.749124	0.183858
O	O38	0.236507	0.241842	0.963498
O	O39	0.518873	0.185073	0.807135
O	O40	0.045010	0.960383	0.173563
O	O41	0.932609	0.093701	0.520802
O	O42	0.901374	0.576623	0.291607
O	O43	0.187894	0.519777	0.139978
O	O44	0.699177	0.934752	0.504698
O	O45	0.578304	0.699423	0.841855
O	O46	0.091143	0.170346	0.629794
O	O47	0.141421	0.515949	0.471319
O	O48	0.365470	0.261564	0.838602
O	O49	0.249247	0.032901	0.181879
O	O50	0.754265	0.504924	0.957805
O	O51	0.807987	0.844991	0.799693
O	O52	0.034554	0.594210	0.171332
O	O53	0.916690	0.355583	0.520716
O	O54	0.422655	0.838969	0.295939
O	O55	0.479007	0.180584	0.136937
O	O56	0.891663	0.699482	0.443839
O	O57	0.691707	0.611800	0.089360
O	O58	0.162146	0.578910	0.314939
O	O59	0.498291	0.856785	0.474908
O	O60	0.580384	0.053635	0.760522
O	O61	0.361061	0.949236	0.426695
O	O62	0.823618	0.918491	0.647235
O	O63	0.166657	0.196006	0.808598
O	O64	0.252007	0.386949	0.104669
O	O65	0.021257	0.277329	0.756376
O	O66	0.493737	0.245845	0.981264
O	O67	0.836894	0.526599	0.135556
O	O68	0.272845	0.713419	0.436241
O	O69	0.387082	0.590369	0.095967
O	O70	0.419278	0.101694	0.313566
O	O71	0.126587	0.142953	0.472230
O	O72	0.938858	0.045299	0.771167
O	O73	0.055697	0.912140	0.422682
O	O74	0.090500	0.436963	0.648853
O	O75	0.796568	0.486405	0.799764
O	O76	0.609084	0.378992	0.101539
O	O77	0.717198	0.257195	0.758244
O	O78	0.743192	0.763503	0.976620
O	O79	0.467147	0.819590	0.139160

O	O80	0.286119	0.079655	0.436229
O	O81	0.404799	0.307485	0.096613
O	O82	0.886458	0.819411	0.308309
O	O83	0.846557	0.480760	0.465032
O	O84	0.951183	0.410904	0.767140
O	O85	0.069448	0.643499	0.424946
O	O86	0.560270	0.176794	0.647994
O	O87	0.504251	0.828533	0.809569
O	O88	0.619890	0.743223	0.105665
O	O89	0.734202	0.974184	0.766471
O	O90	0.232692	0.500930	0.983521
O	O91	0.175081	0.159070	0.140562
Al	Al92	0.929205	0.603935	0.405270
Al	Al93	0.596310	0.938450	0.742055
Al	Al94	0.265998	0.272523	0.076615
Al	Al95	0.388517	0.840685	0.407888
Al	Al96	0.054745	0.171752	0.741040
Al	Al97	0.724051	0.506210	0.071258
Al	Al98	0.151021	0.050904	0.408028
Al	Al99	0.822595	0.395023	0.738173
Al	Al100	0.491784	0.728637	0.076072
Al	Al101	0.058746	0.399781	0.536648
Al	Al102	0.715883	0.731951	0.864511
Al	Al103	0.387016	0.066636	0.201387
Al	Al104	0.592378	0.166322	0.537007
Al	Al105	0.262121	0.499947	0.870658
Al	Al106	0.928712	0.831438	0.200423
Al	Al107	0.829607	0.952192	0.533440
Al	Al108	0.493509	0.276243	0.868795
Al	Al109	0.162703	0.610744	0.202132
Si	Si110	0.923355	0.827294	0.410691
P	P111	0.058236	0.173664	0.532685
P	P112	0.719943	0.505560	0.861258
P	P113	0.389907	0.839930	0.198625
P	P114	0.826010	0.387565	0.529294
P	P115	0.487407	0.728468	0.864176
P	P116	0.156176	0.060717	0.198955
P	P117	0.595040	0.935980	0.534358
P	P118	0.266022	0.273977	0.865912
P	P119	0.934326	0.607505	0.193987
P	P120	0.594505	0.168233	0.743377
P	P121	0.265218	0.499777	0.080682
P	P122	0.160721	0.613029	0.411551
P	P123	0.826177	0.946217	0.745603

P	P124	0.496314	0.278183	0.078959
P	P125	0.386596	0.069286	0.410857
P	P126	0.052528	0.399538	0.744658
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TS-Ethylation-TME-C2H5Z-Si-AlPO-34

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H	H4	0.579657	0.632006	0.328033
H	H5	0.524251	0.676897	0.413749
H	H6	0.514311	0.358651	0.416338
H	H7	0.574124	0.456951	0.329263
H	H8	0.429125	0.377319	0.339666
H	H9	0.710638	0.684039	0.620662
H	H10	0.823823	0.661801	0.608322
H	H11	0.692143	0.546146	0.626246
H	H12	0.369181	0.343227	0.579594
H	H13	0.489134	0.422202	0.643595
H	H14	0.494906	0.351669	0.547433
H	H15	0.488443	0.660866	0.541459
H	H16	0.505581	0.599927	0.639127
H	H17	0.374253	0.544108	0.589683
C	C18	0.459576	0.399553	0.575281
C	C19	0.463497	0.582397	0.574740
C	C20	0.735237	0.626922	0.593239
C	C21	0.720304	0.615566	0.496293

C	C22	0.483040	0.501267	0.522257
C	C23	0.504598	0.510987	0.432862
C	C24	0.512141	0.604507	0.376566
C	C25	0.506627	0.420923	0.378118
O	O26	0.086461	0.293942	0.515220
O	O27	0.300672	0.399083	0.856276
O	O28	0.826549	0.431557	0.631394
O	O29	0.488452	0.153262	0.475550
O	O30	0.734238	0.620277	0.841317
O	O31	0.967641	0.730522	0.182166
O	O32	0.495681	0.759700	0.969536
O	O33	0.150071	0.477764	0.814755
O	O34	0.407077	0.955726	0.181583
O	O35	0.620770	0.058329	0.531538
O	O36	0.162520	0.097001	0.302849
O	O37	0.825742	0.816532	0.134235
O	O38	0.716701	0.291222	0.513466
O	O39	0.602396	0.416777	0.853821
O	O40	0.569055	0.899967	0.637687
O	O41	0.855990	0.865131	0.479557
O	O42	0.378044	0.631996	0.846723
O	O43	0.271969	0.752006	0.190687
O	O44	0.242062	0.246949	0.970179
O	O45	0.522974	0.187987	0.813871
O	O46	0.048574	0.963432	0.180964
O	O47	0.935846	0.095733	0.531009
O	O48	0.904775	0.579469	0.298510
O	O49	0.191707	0.522875	0.146310
O	O50	0.703087	0.936821	0.512544
O	O51	0.581958	0.702226	0.848062
O	O52	0.097988	0.176156	0.636722
O	O53	0.144001	0.518544	0.478334
O	O54	0.369878	0.264975	0.844826
O	O55	0.252787	0.035180	0.188318
O	O56	0.757752	0.510866	0.964869
O	O57	0.812793	0.849028	0.808964
O	O58	0.038518	0.597195	0.178639
O	O59	0.919770	0.358314	0.529858
O	O60	0.426346	0.841905	0.302898
O	O61	0.482729	0.183225	0.143916
O	O62	0.894373	0.701830	0.450277
O	O63	0.694628	0.613931	0.099565
O	O64	0.166570	0.581804	0.321834
O	O65	0.502703	0.859907	0.481457

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O	O69	0.170620	0.198611	0.815854
O	O70	0.256174	0.389898	0.112550
O	O71	0.025358	0.280202	0.763988
O	O72	0.496797	0.248342	0.988168
O	O73	0.841029	0.529449	0.142251
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O	O75	0.391117	0.593257	0.103105
O	O76	0.422191	0.103884	0.320537
O	O77	0.128439	0.144042	0.479089
O	O78	0.943220	0.048020	0.776182
O	O79	0.059852	0.914314	0.427666
O	O80	0.096727	0.439067	0.655534
O	O81	0.801584	0.489543	0.807987
O	O82	0.613423	0.381288	0.108137
O	O83	0.721219	0.261041	0.764105
O	O84	0.745029	0.762118	0.983787
O	O85	0.471058	0.822439	0.146137
O	O86	0.289880	0.082598	0.443706
O	O87	0.409218	0.310815	0.104087
O	O88	0.888771	0.821353	0.314862
O	O89	0.851372	0.483634	0.471209
O	O90	0.955412	0.414097	0.771806
O	O91	0.074234	0.647608	0.431098
O	O92	0.563380	0.177923	0.654739
O	O93	0.508376	0.831798	0.816515
O	O94	0.623797	0.746452	0.113051
O	O95	0.738533	0.976946	0.772561
O	O96	0.237285	0.502874	0.990305
O	O97	0.179161	0.161657	0.146750
Al	Al98	0.933714	0.607221	0.412097
Al	Al99	0.600623	0.941687	0.748972
Al	Al100	0.270471	0.275860	0.083599
Al	Al101	0.392390	0.843448	0.414916
Al	Al102	0.059246	0.174991	0.747795
Al	Al103	0.727747	0.509344	0.078593
Al	Al104	0.154884	0.053675	0.414512
Al	Al105	0.826648	0.399023	0.744486
Al	Al106	0.495680	0.731522	0.083000
Al	Al107	0.062009	0.402039	0.543518
Al	Al108	0.719271	0.734025	0.871140
Al	Al109	0.390576	0.069198	0.208260

Al	Al110	0.596434	0.169046	0.543735
Al	Al111	0.266092	0.502905	0.877222
Al	Al112	0.932254	0.834234	0.207174
Al	Al113	0.833215	0.953663	0.541583
Al	Al114	0.497555	0.279020	0.875595
Al	Al115	0.166727	0.613604	0.209055
Si	Si116	0.927197	0.830197	0.416978
P	P117	0.061723	0.176265	0.540026
P	P118	0.723911	0.509058	0.867803
P	P119	0.393779	0.842800	0.205538
P	P120	0.829589	0.391268	0.536672
P	P121	0.491295	0.731435	0.870818
P	P122	0.160194	0.063633	0.205624
P	P123	0.599227	0.939217	0.541122
P	P124	0.270557	0.277546	0.872268
P	P125	0.938163	0.610403	0.200932
P	P126	0.598686	0.171178	0.750155
P	P127	0.269347	0.502506	0.087714
P	P128	0.164858	0.615961	0.418385
P	P129	0.830177	0.948187	0.752525
P	P130	0.500213	0.280874	0.085928
P	P131	0.390124	0.071899	0.417967
P	P132	0.056926	0.402368	0.751207
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TS-HT-ZCH3-C4-1-Si-AlPO-34

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H	H5	0.594942	0.573231	0.687287
H	H6	0.544814	0.655142	0.635711
H	H7	0.514830	0.432221	0.564487
H	H8	0.442988	0.592520	0.484291
H	H9	0.377458	0.348525	0.447288
H	H10	0.317648	0.428108	0.396155
H	H11	0.614160	0.566763	0.525994
C	C12	0.727831	0.624456	0.492283
C	C13	0.529907	0.570596	0.645069
C	C14	0.522846	0.514422	0.557181
C	C15	0.445336	0.515500	0.490524
C	C16	0.377384	0.426490	0.441561
O	O17	0.085585	0.306604	0.501353
O	O18	0.301299	0.413553	0.844596
O	O19	0.150961	0.492508	0.802129
O	O20	0.161277	0.108828	0.290822
O	O21	0.097156	0.189983	0.623785
O	O22	0.371458	0.280317	0.832600
O	O23	0.253908	0.049089	0.176786
O	O24	0.483370	0.197761	0.131461
O	O25	0.172347	0.213703	0.802071
O	O26	0.256899	0.403762	0.098653
O	O27	0.026039	0.294877	0.751597
O	O28	0.423993	0.116399	0.308001
O	O29	0.131475	0.159375	0.466741
O	O30	0.100416	0.453340	0.642576
O	O31	0.291149	0.096444	0.430230
O	O32	0.410425	0.325203	0.089425
O	O33	0.181351	0.176462	0.135274
O	O34	0.735502	0.634890	0.830870
O	O35	0.969528	0.744909	0.167871
O	O36	0.825647	0.829987	0.124414
O	O37	0.569553	0.912425	0.625487
O	O38	0.853475	0.875030	0.467128
O	O39	0.908639	0.595581	0.285439
O	O40	0.704227	0.951371	0.500501
O	O41	0.584052	0.717723	0.839141
O	O42	0.814086	0.863398	0.796290
O	O43	0.897886	0.715345	0.438947
O	O44	0.696653	0.628414	0.084707
O	O45	0.503178	0.871001	0.469256

O	O46	0.828000	0.931497	0.642124
O	O47	0.842031	0.543335	0.130065
O	O48	0.893904	0.835470	0.303137
O	O49	0.851634	0.495190	0.456037
O	O50	0.509841	0.846001	0.803991
O	O51	0.624670	0.759961	0.098944
O	O52	0.739696	0.991097	0.759494
O	O53	0.825444	0.446668	0.617111
O	O54	0.489614	0.168919	0.462962
O	O55	0.618288	0.069727	0.518944
O	O56	0.718982	0.302892	0.500385
O	O57	0.603962	0.431368	0.841830
O	O58	0.524732	0.202923	0.800733
O	O59	0.937114	0.107494	0.516078
O	O60	0.922178	0.373721	0.519026
O	O61	0.587588	0.072190	0.755085
O	O62	0.944241	0.062513	0.763841
O	O63	0.802591	0.504633	0.794163
O	O64	0.614550	0.395335	0.094453
O	O65	0.723028	0.276174	0.750687
O	O66	0.957148	0.429929	0.756356
O	O67	0.564868	0.192882	0.641688
O	O68	0.494929	0.775722	0.957787
O	O69	0.760599	0.523747	0.952134
O	O70	0.750804	0.780516	0.972051
O	O71	0.408405	0.970026	0.167837
O	O72	0.380011	0.646142	0.834811
O	O73	0.273379	0.766373	0.177618
O	O74	0.049893	0.977597	0.167122
O	O75	0.193020	0.536522	0.134484
O	O76	0.146709	0.531350	0.464488
O	O77	0.040129	0.611371	0.164484
O	O78	0.426668	0.857355	0.290601
O	O79	0.167346	0.596421	0.308828
O	O80	0.367260	0.966528	0.423387
O	O81	0.278577	0.729423	0.430969
O	O82	0.391878	0.607237	0.089489
O	O83	0.060345	0.928725	0.419282
O	O84	0.472916	0.836526	0.134793
O	O85	0.075465	0.660092	0.420154
O	O86	0.241524	0.259529	0.957215
O	O87	0.498228	0.261148	0.975136
O	O88	0.236780	0.517573	0.977778
Al	Al89	0.271314	0.289633	0.070527

Al	Al90	0.059839	0.189530	0.735055
Al	Al91	0.155634	0.067078	0.402716
Al	Al92	0.064222	0.416208	0.530856
Al	Al93	0.391939	0.083256	0.195596
Al	Al94	0.498976	0.293382	0.862994
Al	Al95	0.935705	0.620330	0.399293
Al	Al96	0.601802	0.955974	0.736359
Al	Al97	0.496540	0.745726	0.070698
Al	Al98	0.721917	0.749738	0.860098
Al	Al99	0.934390	0.848295	0.194781
Al	Al100	0.833660	0.966210	0.528737
Al	Al101	0.729373	0.523301	0.065614
Al	Al102	0.827783	0.414408	0.730274
Al	Al103	0.597109	0.182474	0.530734
Al	Al104	0.393770	0.857361	0.402927
Al	Al105	0.266723	0.517628	0.865041
Al	Al106	0.168119	0.628072	0.195996
Si	Si107	0.928500	0.843062	0.405961
P	P108	0.062329	0.189638	0.526680
P	P109	0.161107	0.077373	0.193342
P	P110	0.271332	0.291821	0.859690
P	P111	0.270020	0.516577	0.074799
P	P112	0.391876	0.086011	0.405578
P	P113	0.058586	0.417229	0.737917
P	P114	0.725737	0.523400	0.855618
P	P115	0.599172	0.951500	0.528787
P	P116	0.940224	0.625037	0.187467
P	P117	0.831479	0.962433	0.739801
P	P118	0.724990	0.749713	0.070349
P	P119	0.830550	0.404749	0.523236
P	P120	0.600456	0.186129	0.737005
P	P121	0.501335	0.294859	0.072578
P	P122	0.395024	0.857357	0.192943
P	P123	0.492555	0.746470	0.859563
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TS-HT-ZCH3-C5-Si-AlPO-34

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H	H2	0.760707	0.608479	0.546361
H	H3	0.704627	0.572449	0.431082
H	H4	0.453749	0.552733	0.670130
H	H5	0.596925	0.597462	0.679001
H	H6	0.552041	0.677172	0.617012
H	H7	0.457627	0.612462	0.474156
H	H8	0.361397	0.362017	0.438769
H	H9	0.322272	0.457509	0.386339
H	H10	0.613106	0.572722	0.520087
H	H11	0.568742	0.416572	0.620285
H	H12	0.509229	0.366184	0.514328
H	H13	0.423969	0.358172	0.604439
C	C14	0.505486	0.409520	0.573407
C	C15	0.730041	0.628233	0.487263
C	C16	0.533010	0.592914	0.634224
C	C17	0.522172	0.524044	0.552127
C	C18	0.449340	0.530660	0.482445
C	C19	0.374808	0.445725	0.433154
O	O20	0.084317	0.303750	0.501400
O	O21	0.300772	0.410958	0.843827
O	O22	0.151341	0.491198	0.802431
O	O23	0.162139	0.107615	0.291121
O	O24	0.099153	0.189638	0.624410
O	O25	0.371836	0.278445	0.832978
O	O26	0.253781	0.046739	0.177101
O	O27	0.483228	0.194567	0.131509
O	O28	0.172605	0.210489	0.802634
O	O29	0.257203	0.401386	0.099719
O	O30	0.026941	0.292822	0.753312
O	O31	0.423711	0.113303	0.308388
O	O32	0.128270	0.154828	0.467134
O	O33	0.099608	0.450006	0.643263
O	O34	0.292573	0.096374	0.431056

O	O35	0.410441	0.322173	0.089596
O	O36	0.181049	0.173847	0.135164
O	O37	0.735942	0.632984	0.829916
O	O38	0.968421	0.742135	0.168227
O	O39	0.824988	0.828167	0.125810
O	O40	0.569175	0.915816	0.626391
O	O41	0.858539	0.876637	0.467982
O	O42	0.907896	0.593458	0.286302
O	O43	0.702554	0.943328	0.503044
O	O44	0.584434	0.715241	0.840950
O	O45	0.815065	0.862468	0.799647
O	O46	0.898089	0.713873	0.439621
O	O47	0.696311	0.625555	0.089010
O	O48	0.502765	0.869576	0.470522
O	O49	0.827925	0.926132	0.644040
O	O50	0.841964	0.540144	0.130915
O	O51	0.894165	0.833641	0.303907
O	O52	0.852019	0.494255	0.457446
O	O53	0.510341	0.843022	0.803994
O	O54	0.624067	0.757222	0.099426
O	O55	0.740322	0.988848	0.759576
O	O56	0.826789	0.446811	0.618646
O	O57	0.490490	0.164366	0.463192
O	O58	0.624825	0.069686	0.514693
O	O59	0.718073	0.302853	0.502693
O	O60	0.604294	0.429674	0.842722
O	O61	0.524432	0.202027	0.799274
O	O62	0.935619	0.105547	0.520274
O	O63	0.921029	0.371380	0.520240
O	O64	0.589418	0.070679	0.761373
O	O65	0.944886	0.060461	0.763710
O	O66	0.803356	0.502146	0.796630
O	O67	0.614523	0.392185	0.094869
O	O68	0.722736	0.274528	0.749899
O	O69	0.956960	0.426969	0.757573
O	O70	0.564009	0.182902	0.641868
O	O71	0.494665	0.774014	0.958414
O	O72	0.760054	0.523972	0.953489
O	O73	0.750619	0.774737	0.973728
O	O74	0.407484	0.966860	0.168131
O	O75	0.380391	0.643646	0.835661
O	O76	0.273449	0.763187	0.179400
O	O77	0.049791	0.975368	0.168115
O	O78	0.192254	0.533704	0.134394

O	O79	0.145107	0.528972	0.465705
O	O80	0.040161	0.609459	0.165851
O	O81	0.427601	0.856068	0.291520
O	O82	0.166685	0.592113	0.309508
O	O83	0.364547	0.962765	0.423583
O	O84	0.278799	0.726112	0.430831
O	O85	0.391372	0.604891	0.089807
O	O86	0.063349	0.926070	0.417950
O	O87	0.472817	0.833919	0.135768
O	O88	0.076079	0.658874	0.419582
O	O89	0.241992	0.258262	0.957524
O	O90	0.498498	0.258418	0.975207
O	O91	0.236521	0.513903	0.978057
Al	Al92	0.271505	0.287348	0.070916
Al	Al93	0.060590	0.187607	0.735634
Al	Al94	0.156619	0.065486	0.402915
Al	Al95	0.063075	0.413332	0.531577
Al	Al96	0.391652	0.080421	0.195942
Al	Al97	0.499327	0.291590	0.863216
Al	Al98	0.935996	0.618597	0.399982
Al	Al99	0.602450	0.954714	0.737969
Al	Al100	0.496134	0.743340	0.071204
Al	Al101	0.722227	0.747055	0.861488
Al	Al102	0.934171	0.846099	0.195432
Al	Al103	0.834107	0.963296	0.531185
Al	Al104	0.728979	0.520900	0.067180
Al	Al105	0.828212	0.412791	0.731461
Al	Al106	0.598663	0.178890	0.530562
Al	Al107	0.393298	0.854922	0.403660
Al	Al108	0.266782	0.515158	0.865276
Al	Al109	0.167798	0.624910	0.196854
Si	Si110	0.930974	0.842378	0.406153
P	P111	0.061428	0.187230	0.527848
P	P112	0.161190	0.075287	0.193738
P	P113	0.271530	0.289645	0.859856
P	P114	0.269699	0.513776	0.075197
P	P115	0.391691	0.083153	0.406028
P	P116	0.058644	0.414825	0.738872
P	P117	0.725914	0.521897	0.856535
P	P118	0.600166	0.949999	0.528974
P	P119	0.939792	0.622544	0.188300
P	P120	0.832016	0.959747	0.741146
P	P121	0.724458	0.746402	0.072283
P	P122	0.830473	0.403911	0.524887

P	P123	0.600591	0.182732	0.737994
P	P124	0.501339	0.291815	0.072742
P	P125	0.394996	0.854774	0.193948
P	P126	0.492822	0.744055	0.860384
P	P127	0.166108	0.626630	0.406109

TS-HT-ZC2H5-C4-1-Si-AlPO-34

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H	H2	0.563409	0.572983	0.672240
H	H3	0.515850	0.656189	0.619392
H	H4	0.479690	0.430091	0.550110
H	H5	0.410722	0.592207	0.470927
H	H6	0.359909	0.356375	0.418876
H	H7	0.300800	0.437413	0.369253
H	H8	0.580901	0.562357	0.511169
H	H9	0.713488	0.693271	0.472497
H	H10	0.568980	0.537537	0.362276
H	H11	0.664751	0.487662	0.357338
H	H12	0.700457	0.624510	0.318523
H	H13	0.723482	0.570618	0.506664
C	C14	0.498996	0.571054	0.629410
C	C15	0.492064	0.513949	0.541543
C	C16	0.416372	0.516733	0.473843
C	C17	0.356890	0.433072	0.417068
C	C18	0.657345	0.561101	0.369585
C	C19	0.697635	0.610064	0.457644
O	O20	0.082294	0.301289	0.503135

O	O21	0.301718	0.410570	0.844437
O	O22	0.151477	0.489787	0.803548
O	O23	0.164236	0.108788	0.291768
O	O24	0.098477	0.187460	0.625604
O	O25	0.371618	0.276855	0.834456
O	O26	0.255359	0.046390	0.178356
O	O27	0.484698	0.194551	0.133190
O	O28	0.172346	0.209886	0.804481
O	O29	0.258846	0.401136	0.102362
O	O30	0.027036	0.291839	0.753661
O	O31	0.424609	0.114196	0.310195
O	O32	0.131049	0.156123	0.468193
O	O33	0.099910	0.449563	0.644067
O	O34	0.290169	0.091980	0.431878
O	O35	0.411594	0.322119	0.091971
O	O36	0.181873	0.172578	0.135391
O	O37	0.734954	0.631112	0.828270
O	O38	0.968239	0.740832	0.172718
O	O39	0.828682	0.828851	0.122205
O	O40	0.568708	0.912089	0.627618
O	O41	0.851984	0.869069	0.469151
O	O42	0.908797	0.587073	0.286443
O	O43	0.703633	0.945694	0.504054
O	O44	0.583341	0.713600	0.838086
O	O45	0.815029	0.861688	0.801126
O	O46	0.897336	0.712036	0.434128
O	O47	0.697375	0.624972	0.092937
O	O48	0.503196	0.867919	0.471506
O	O49	0.827707	0.925369	0.645349
O	O50	0.843984	0.540161	0.130227
O	O51	0.888674	0.834200	0.303078
O	O52	0.851095	0.493613	0.459253
O	O53	0.509574	0.842764	0.805831
O	O54	0.626025	0.757378	0.102638
O	O55	0.739929	0.987679	0.761001
O	O56	0.825092	0.443178	0.619961
O	O57	0.488480	0.163879	0.465716
O	O58	0.620994	0.067639	0.518144
O	O59	0.717637	0.301170	0.502359
O	O60	0.604081	0.427941	0.842982
O	O61	0.524327	0.199666	0.802086
O	O62	0.936633	0.101346	0.519695
O	O63	0.920843	0.370641	0.520541
O	O64	0.588585	0.069152	0.760104

O	O65	0.944580	0.059553	0.765197
O	O66	0.803838	0.500635	0.798411
O	O67	0.615761	0.392202	0.096871
O	O68	0.722970	0.272994	0.752980
O	O69	0.957257	0.426122	0.758494
O	O70	0.565122	0.186224	0.643789
O	O71	0.498336	0.772727	0.959329
O	O72	0.758794	0.524737	0.954031
O	O73	0.745143	0.768296	0.973375
O	O74	0.410189	0.967319	0.170690
O	O75	0.379463	0.643440	0.837602
O	O76	0.274758	0.763727	0.179955
O	O77	0.051390	0.974374	0.169898
O	O78	0.194615	0.534158	0.135960
O	O79	0.145801	0.526873	0.465897
O	O80	0.042383	0.610315	0.164973
O	O81	0.428415	0.853559	0.292630
O	O82	0.167767	0.592160	0.310178
O	O83	0.366265	0.962138	0.423909
O	O84	0.279143	0.724738	0.432332
O	O85	0.393322	0.604406	0.090759
O	O86	0.058563	0.926235	0.416886
O	O87	0.473910	0.833532	0.136300
O	O88	0.076028	0.656642	0.421143
O	O89	0.243060	0.259019	0.959015
O	O90	0.499321	0.258862	0.976979
O	O91	0.237495	0.512154	0.979712
Al	Al92	0.272677	0.287096	0.072355
Al	Al93	0.060503	0.186345	0.736835
Al	Al94	0.155325	0.064397	0.403377
Al	Al95	0.062547	0.411957	0.532491
Al	Al96	0.393200	0.080406	0.197758
Al	Al97	0.499277	0.290282	0.864570
Al	Al98	0.936053	0.617002	0.400281
Al	Al99	0.602100	0.953154	0.738806
Al	Al100	0.498198	0.743004	0.072428
Al	Al101	0.720544	0.744477	0.860336
Al	Al102	0.934172	0.845926	0.196130
Al	Al103	0.833072	0.959821	0.531898
Al	Al104	0.729921	0.520760	0.067977
Al	Al105	0.827972	0.411119	0.732887
Al	Al106	0.597447	0.178792	0.532432
Al	Al107	0.393872	0.853505	0.404676
Al	Al108	0.266884	0.514076	0.866619

Al	Al109	0.169317	0.625376	0.197558
Si	Si110	0.926629	0.839190	0.405318
P	P111	0.061535	0.185258	0.528828
P	P112	0.162642	0.074854	0.194759
P	P113	0.271910	0.289160	0.861079
P	P114	0.271417	0.513324	0.076804
P	P115	0.391228	0.082029	0.407463
P	P116	0.058837	0.413909	0.739682
P	P117	0.725415	0.520804	0.856577
P	P118	0.599655	0.948845	0.530623
P	P119	0.940977	0.620929	0.189185
P	P120	0.831791	0.958794	0.742423
P	P121	0.724890	0.745089	0.072889
P	P122	0.829712	0.402399	0.525727
P	P123	0.600722	0.182235	0.739599
P	P124	0.502499	0.291839	0.074589
P	P125	0.396526	0.854361	0.195118
P	P126	0.492986	0.743131	0.860842
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TS-HT-ZC3H7-C5-Si-AlPO-34

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H	H3	0.450291	0.598585	0.665121
H	H4	0.424096	0.665937	0.576099
H	H5	0.406886	0.597079	0.421873
H	H6	0.335825	0.348951	0.408426

H	H7	0.323582	0.438230	0.323848
H	H8	0.530874	0.575609	0.530096
H	H9	0.454168	0.421630	0.640687
H	H10	0.445973	0.366718	0.533017
H	H11	0.326011	0.353976	0.584067
H	H12	0.800272	0.624272	0.580945
H	H13	0.669937	0.501870	0.596304
H	H14	0.693022	0.637581	0.628511
H	H15	0.646891	0.454460	0.429339
H	H16	0.693173	0.572444	0.355349
H	H17	0.560957	0.511844	0.399601
C	C18	0.709411	0.589767	0.579266
C	C19	0.647293	0.531734	0.415958
C	C20	0.415401	0.409659	0.575400
C	C21	0.685534	0.610415	0.489022
C	C22	0.405607	0.585247	0.602535
C	C23	0.438220	0.521299	0.537185
C	C24	0.396112	0.517966	0.445148
C	C25	0.350845	0.430690	0.389639
O	O26	0.086676	0.299901	0.508980
O	O27	0.304702	0.406773	0.847149
O	O28	0.155501	0.486474	0.805402
O	O29	0.166695	0.107736	0.294753
O	O30	0.099646	0.182257	0.629586
O	O31	0.373391	0.272224	0.837452
O	O32	0.256884	0.043166	0.182355
O	O33	0.486580	0.190267	0.136761
O	O34	0.174292	0.205782	0.808243
O	O35	0.260967	0.397436	0.106701
O	O36	0.029603	0.287868	0.757363
O	O37	0.427471	0.109886	0.313472
O	O38	0.136267	0.156496	0.471998
O	O39	0.094535	0.445284	0.648075
O	O40	0.293675	0.091464	0.434460
O	O41	0.412704	0.317393	0.096470
O	O42	0.181956	0.167498	0.137436
O	O43	0.736784	0.627369	0.833189
O	O44	0.970643	0.736471	0.177079
O	O45	0.829578	0.823299	0.127652
O	O46	0.572876	0.911539	0.630039
O	O47	0.854197	0.865237	0.473827
O	O48	0.904533	0.582577	0.291605
O	O49	0.707070	0.944164	0.506088
O	O50	0.585390	0.709645	0.842119

O	O51	0.816307	0.856360	0.802634
O	O52	0.906588	0.712755	0.441970
O	O53	0.698295	0.620635	0.093626
O	O54	0.507037	0.869145	0.474061
O	O55	0.829990	0.924005	0.648203
O	O56	0.845432	0.536260	0.134071
O	O57	0.891302	0.828895	0.308569
O	O58	0.859862	0.494003	0.466392
O	O59	0.511236	0.837996	0.807778
O	O60	0.627384	0.753244	0.105677
O	O61	0.741650	0.983612	0.765427
O	O62	0.833299	0.438334	0.625627
O	O63	0.491014	0.160520	0.469085
O	O64	0.627446	0.068565	0.521555
O	O65	0.717558	0.303038	0.506779
O	O66	0.605539	0.423979	0.846723
O	O67	0.525803	0.195405	0.806111
O	O68	0.940236	0.099305	0.521341
O	O69	0.918697	0.359782	0.521321
O	O70	0.589654	0.064716	0.764026
O	O71	0.946283	0.055318	0.769775
O	O72	0.804674	0.497031	0.800634
O	O73	0.617111	0.388180	0.100415
O	O74	0.724509	0.268363	0.757891
O	O75	0.958492	0.420536	0.768940
O	O76	0.567547	0.182991	0.647840
O	O77	0.502121	0.771917	0.962624
O	O78	0.761105	0.519109	0.957412
O	O79	0.749252	0.768149	0.977202
O	O80	0.410041	0.962394	0.173318
O	O81	0.381624	0.639875	0.842970
O	O82	0.274795	0.758838	0.183698
O	O83	0.052528	0.969904	0.174966
O	O84	0.195755	0.530254	0.138471
O	O85	0.143764	0.524788	0.471765
O	O86	0.041889	0.603206	0.174080
O	O87	0.428570	0.850034	0.296208
O	O88	0.175133	0.587165	0.314574
O	O89	0.366523	0.958723	0.428171
O	O90	0.282778	0.721004	0.437238
O	O91	0.394293	0.600663	0.092011
O	O92	0.061727	0.927171	0.421426
O	O93	0.474100	0.828463	0.140280
O	O94	0.081478	0.657200	0.418288

O	O95	0.245889	0.256136	0.962426
O	O96	0.500315	0.254827	0.980802
O	O97	0.237070	0.505069	0.982620
Al	Al98	0.274144	0.283071	0.076016
Al	Al99	0.062297	0.181888	0.740837
Al	Al100	0.158780	0.064148	0.406504
Al	Al101	0.061536	0.407455	0.536011
Al	Al102	0.394508	0.076203	0.201166
Al	Al103	0.500879	0.286166	0.868444
Al	Al104	0.939962	0.616297	0.404401
Al	Al105	0.604191	0.949511	0.741886
Al	Al106	0.499754	0.739518	0.075550
Al	Al107	0.722831	0.741297	0.864612
Al	Al108	0.935641	0.840894	0.201427
Al	Al109	0.836350	0.958065	0.534431
Al	Al110	0.731588	0.516442	0.071350
Al	Al111	0.830696	0.405980	0.738891
Al	Al112	0.600221	0.177308	0.536198
Al	Al113	0.395348	0.850986	0.408439
Al	Al114	0.269341	0.509668	0.869907
Al	Al115	0.170762	0.620032	0.202490
Si	Si116	0.930644	0.836212	0.410773
P	P117	0.064857	0.183001	0.532545
P	P118	0.163810	0.071278	0.198302
P	P119	0.274275	0.285333	0.864348
P	P120	0.272362	0.508794	0.079641
P	P121	0.393450	0.079128	0.410814
P	P122	0.059530	0.409525	0.744638
P	P123	0.726979	0.516555	0.860374
P	P124	0.604067	0.948872	0.533178
P	P125	0.940848	0.616005	0.194833
P	P126	0.833575	0.955159	0.745809
P	P127	0.726785	0.741566	0.076351
P	P128	0.833364	0.398971	0.529996
P	P129	0.602263	0.178006	0.743764
P	P130	0.503861	0.287635	0.078521
P	P131	0.396540	0.849723	0.198570
P	P132	0.495383	0.739925	0.864579
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TS-C6-Cyclization-Si-AlPO-34

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H	H3	0.515817	0.432090	0.356160
H	H4	0.748641	0.561255	0.528466
H	H5	0.597704	0.402812	0.428151
H	H6	0.567805	0.423239	0.612825
H	H7	0.432235	0.478740	0.481858
H	H8	0.417662	0.345891	0.500543
H	H9	0.705340	0.589918	0.359377
H	H10	0.618161	0.633758	0.405458
H	H11	0.751339	0.695254	0.526739
C	C12	0.574092	0.577739	0.615864
C	C13	0.541508	0.476593	0.580520
C	C14	0.560170	0.455284	0.419520
C	C15	0.477912	0.435052	0.496045
C	C16	0.652121	0.578587	0.416840
C	C17	0.724900	0.615635	0.496219
O	O18	0.087969	0.293997	0.504813
O	O19	0.302087	0.399142	0.847805
O	O20	0.826804	0.432324	0.620649
O	O21	0.490566	0.155193	0.465684
O	O22	0.734832	0.620681	0.830737
O	O23	0.969143	0.731445	0.171588
O	O24	0.495984	0.760370	0.959596
O	O25	0.151690	0.478246	0.805013
O	O26	0.408387	0.956485	0.171394
O	O27	0.619912	0.056668	0.521931
O	O28	0.163689	0.097125	0.293617
O	O29	0.827039	0.817908	0.125563
O	O30	0.719220	0.289986	0.503383

O	O31	0.604022	0.416942	0.842708
O	O32	0.570489	0.898691	0.627827
O	O33	0.857183	0.864524	0.470224
O	O34	0.380651	0.632202	0.836134
O	O35	0.273506	0.752759	0.181245
O	O36	0.242698	0.245610	0.960550
O	O37	0.524849	0.188230	0.803889
O	O38	0.050351	0.964530	0.171152
O	O39	0.937805	0.095732	0.521200
O	O40	0.905739	0.580738	0.288291
O	O41	0.193196	0.523654	0.136085
O	O42	0.705180	0.937804	0.502816
O	O43	0.584862	0.704337	0.839346
O	O44	0.099643	0.177136	0.627044
O	O45	0.146075	0.519093	0.468293
O	O46	0.371243	0.264993	0.835417
O	O47	0.254510	0.036208	0.178909
O	O48	0.758130	0.511833	0.954779
O	O49	0.815332	0.850033	0.799651
O	O50	0.040134	0.598159	0.168916
O	O51	0.922375	0.359180	0.521126
O	O52	0.428603	0.843402	0.292761
O	O53	0.484185	0.184128	0.133947
O	O54	0.896454	0.701729	0.440655
O	O55	0.696682	0.615110	0.090883
O	O56	0.167623	0.581442	0.311646
O	O57	0.504189	0.858243	0.471519
O	O58	0.588462	0.058388	0.757318
O	O59	0.368543	0.953306	0.424575
O	O60	0.827458	0.916491	0.644961
O	O61	0.172117	0.199139	0.805989
O	O62	0.257348	0.390634	0.101283
O	O63	0.026538	0.280764	0.754399
O	O64	0.499611	0.249481	0.978135
O	O65	0.842791	0.530267	0.131908
O	O66	0.278485	0.716519	0.432752
O	O67	0.392722	0.593981	0.093128
O	O68	0.424413	0.104688	0.310683
O	O69	0.130630	0.144241	0.469825
O	O70	0.944822	0.048670	0.765779
O	O71	0.061475	0.914541	0.418655
O	O72	0.099455	0.439444	0.645670
O	O73	0.803714	0.490786	0.798212
O	O74	0.615002	0.382274	0.098486

O	O75	0.723267	0.262480	0.753959
O	O76	0.748802	0.762734	0.974514
O	O77	0.472394	0.823278	0.135910
O	O78	0.291689	0.082428	0.433813
O	O79	0.410844	0.311653	0.093332
O	O80	0.891254	0.821386	0.305471
O	O81	0.852568	0.482341	0.459997
O	O82	0.957433	0.415473	0.760777
O	O83	0.075514	0.647293	0.420885
O	O84	0.565517	0.179615	0.644597
O	O85	0.509976	0.832553	0.806577
O	O86	0.625487	0.747625	0.102034
O	O87	0.740134	0.976948	0.762454
O	O88	0.239226	0.505205	0.980007
O	O89	0.181133	0.163045	0.137856
Al	Al90	0.935319	0.607164	0.402104
Al	Al91	0.602392	0.942001	0.738768
Al	Al92	0.271837	0.276407	0.073683
Al	Al93	0.394634	0.843730	0.404909
Al	Al94	0.060821	0.175824	0.737995
Al	Al95	0.729176	0.510310	0.068748
Al	Al96	0.156570	0.053670	0.405135
Al	Al97	0.828596	0.400557	0.734015
Al	Al98	0.496976	0.732278	0.072929
Al	Al99	0.064787	0.402718	0.533722
Al	Al100	0.722001	0.735417	0.862067
Al	Al101	0.392307	0.070089	0.198418
Al	Al102	0.597893	0.168782	0.533722
Al	Al103	0.268065	0.503664	0.867146
Al	Al104	0.934262	0.835321	0.197610
Al	Al105	0.834977	0.953879	0.531878
Al	Al106	0.499235	0.279332	0.865526
Al	Al107	0.168316	0.614212	0.199085
Si	Si108	0.928977	0.829883	0.407793
P	P109	0.063644	0.176647	0.530261
P	P110	0.725180	0.509737	0.857451
P	P111	0.395375	0.843715	0.195547
P	P112	0.831458	0.391032	0.526467
P	P113	0.493088	0.732339	0.861007
P	P114	0.161896	0.064592	0.196270
P	P115	0.600227	0.938129	0.531232
P	P116	0.271793	0.277420	0.862884
P	P117	0.939732	0.611415	0.190703
P	P118	0.600907	0.172239	0.739924

P	P119	0.270912	0.503608	0.077320
P	P120	0.166402	0.616107	0.408085
P	P121	0.831964	0.948410	0.742562
P	P122	0.501993	0.281789	0.075841
P	P123	0.392583	0.072791	0.408164
P	P124	0.058828	0.403087	0.741169
P	P125	0.725042	0.735961	0.073519

TS-C7-Cyclization-Si-AlPO-34

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H	H4	0.534533	0.548059	0.320716
H	H5	0.732814	0.552299	0.497230
H	H6	0.593949	0.470992	0.361278
H	H7	0.401274	0.345692	0.552332
H	H8	0.512958	0.351446	0.495593
H	H9	0.431809	0.518452	0.465915
H	H10	0.393736	0.398793	0.403209
H	H11	0.717615	0.677896	0.362411
H	H12	0.632613	0.694764	0.437127
H	H13	0.764830	0.689068	0.540558
C	C14	0.557657	0.476973	0.593328
C	C15	0.577208	0.578620	0.617739
C	C16	0.481271	0.404166	0.521148
C	C17	0.562596	0.526375	0.381515
C	C18	0.461676	0.462956	0.442906

C	C19	0.659802	0.636068	0.417763
C	C20	0.727656	0.626919	0.489461
O	O21	0.093360	0.298765	0.507650
O	O22	0.306805	0.403999	0.851458
O	O23	0.833236	0.437165	0.624236
O	O24	0.496795	0.157283	0.468484
O	O25	0.741611	0.626257	0.834576
O	O26	0.974458	0.736559	0.176035
O	O27	0.503315	0.766435	0.963032
O	O28	0.157719	0.483966	0.807425
O	O29	0.414373	0.961266	0.174782
O	O30	0.629274	0.062331	0.524119
O	O31	0.169711	0.101903	0.296734
O	O32	0.832542	0.822616	0.128824
O	O33	0.724210	0.295413	0.506974
O	O34	0.609839	0.422668	0.846737
O	O35	0.576673	0.904941	0.631240
O	O36	0.867551	0.872570	0.474406
O	O37	0.386130	0.637285	0.840685
O	O38	0.279898	0.757494	0.184170
O	O39	0.248555	0.250247	0.963800
O	O40	0.530243	0.194023	0.806266
O	O41	0.056600	0.969929	0.173697
O	O42	0.942592	0.101213	0.526008
O	O43	0.912842	0.584402	0.291134
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O	O46	0.590291	0.708719	0.842471
O	O47	0.106173	0.182836	0.630152
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O	O52	0.821049	0.855580	0.803904
O	O53	0.046724	0.604470	0.170498
O	O54	0.927493	0.364590	0.522791
O	O55	0.434367	0.847893	0.296229
O	O56	0.490229	0.188866	0.136833
O	O57	0.899665	0.706462	0.440684
O	O58	0.702459	0.619752	0.094128
O	O59	0.171494	0.587002	0.314909
O	O60	0.509475	0.863587	0.475114
O	O61	0.593538	0.062979	0.762324
O	O62	0.371575	0.956475	0.426943

O	O63	0.832444	0.920694	0.648900
O	O64	0.177911	0.203909	0.809224
O	O65	0.263554	0.395831	0.104236
O	O66	0.032723	0.285922	0.757921
O	O67	0.504971	0.254136	0.981059
O	O68	0.848984	0.535599	0.134871
O	O69	0.283494	0.721014	0.436138
O	O70	0.398017	0.599236	0.095730
O	O71	0.429747	0.108994	0.313668
O	O72	0.134377	0.147620	0.472822
O	O73	0.950680	0.053856	0.768793
O	O74	0.069617	0.918585	0.420523
O	O75	0.103510	0.443667	0.648501
O	O76	0.809018	0.495324	0.801371
O	O77	0.621024	0.386928	0.101265
O	O78	0.728523	0.266983	0.756779
O	O79	0.753321	0.767629	0.978118
O	O80	0.479045	0.828597	0.139508
O	O81	0.298463	0.088756	0.437301
O	O82	0.416898	0.316573	0.096599
O	O83	0.897537	0.830210	0.308444
O	O84	0.856665	0.487971	0.463829
O	O85	0.962729	0.419849	0.764784
O	O86	0.080118	0.652083	0.425590
O	O87	0.570643	0.181869	0.647504
O	O88	0.515614	0.837072	0.809655
O	O89	0.630720	0.751591	0.106516
O	O90	0.745977	0.982447	0.766108
O	O91	0.243348	0.509773	0.983508
O	O92	0.187221	0.168647	0.141323
Al	Al93	0.939950	0.611649	0.404966
Al	Al94	0.608105	0.947180	0.742461
Al	Al95	0.278011	0.281574	0.076815
Al	Al96	0.399657	0.848113	0.408234
Al	Al97	0.066831	0.180963	0.741140
Al	Al98	0.735150	0.515098	0.071900
Al	Al99	0.163043	0.058705	0.408275
Al	Al100	0.834108	0.405121	0.737448
Al	Al101	0.502959	0.737389	0.076259
Al	Al102	0.069524	0.407253	0.536423
Al	Al103	0.727469	0.740231	0.865545
Al	Al104	0.398235	0.074946	0.201325
Al	Al105	0.604422	0.172694	0.536731
Al	Al106	0.273057	0.508686	0.870693

Al	Al107	0.940345	0.841194	0.200524
Al	Al108	0.841006	0.958760	0.536011
Al	Al109	0.505014	0.284890	0.868573
Al	Al110	0.173964	0.619372	0.202135
Si	Si111	0.936665	0.836781	0.410338
P	P112	0.068776	0.181467	0.533629
P	P113	0.731276	0.514957	0.860970
P	P114	0.401557	0.848589	0.198925
P	P115	0.836577	0.396380	0.529729
P	P116	0.499033	0.737298	0.864526
P	P117	0.168059	0.069884	0.199249
P	P118	0.606558	0.942782	0.534365
P	P119	0.277402	0.282511	0.866165
P	P120	0.945931	0.616473	0.193682
P	P121	0.606139	0.176587	0.743198
P	P122	0.276201	0.508483	0.080555
P	P123	0.171005	0.621017	0.411649
P	P124	0.837560	0.953521	0.746333
P	P125	0.507886	0.286551	0.078803
P	P126	0.397946	0.076810	0.411091
P	P127	0.064227	0.407974	0.744341
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TS-Elimination-C6-C3-H2O-Si-AlPO-34

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H	H3	0.509624	0.378222	0.620874

H	H4	0.610315	0.426131	0.533620
H	H5	0.565309	0.572876	0.661399
H	H6	0.492440	0.707655	0.598708
H	H7	0.373933	0.595622	0.648050
H	H8	0.359831	0.672473	0.561205
H	H9	0.313664	0.313117	0.622922
H	H10	0.383521	0.443183	0.676642
H	H11	0.251433	0.396037	0.631824
H	H12	0.768620	0.674706	0.593166
H	H13	0.696164	0.625671	0.486546
H	H14	0.667575	0.719118	0.553130
H	H15	0.895434	0.791344	0.634219
H	H16	0.316103	0.358422	0.411433
H	H17	0.392948	0.602381	0.383680
H	H18	0.368477	0.299514	0.487257
H	H19	0.460481	0.416090	0.423487
H	H20	0.504422	0.577293	0.393729
H	H21	0.518008	0.703241	0.433352
C	C22	0.591028	0.444267	0.599372
C	C23	0.381976	0.377958	0.460226
C	C24	0.380359	0.452607	0.532277
C	C25	0.601222	0.555584	0.603619
C	C26	0.415663	0.561560	0.516766
C	C27	0.409529	0.636833	0.585356
C	C28	0.460940	0.613908	0.427678
C	C29	0.330282	0.398608	0.620367
C	C30	0.671661	0.643205	0.550340
O	O31	0.082678	0.305082	0.504975
O	O32	0.301286	0.411408	0.846162
O	O33	0.154567	0.491631	0.796479
O	O34	0.169121	0.120882	0.287216
O	O35	0.082695	0.175186	0.621791
O	O36	0.370476	0.277803	0.830730
O	O37	0.253118	0.049963	0.174536
O	O38	0.483089	0.196540	0.129095
O	O39	0.172824	0.213546	0.797255
O	O40	0.257349	0.403079	0.093491
O	O41	0.026464	0.293974	0.747786
O	O42	0.424431	0.117900	0.305664
O	O43	0.124795	0.157113	0.464657
O	O44	0.088592	0.452934	0.640327
O	O45	0.294068	0.102243	0.428803
O	O46	0.408472	0.322068	0.085194
O	O47	0.177270	0.173482	0.129133

O	O48	0.736447	0.633830	0.829006
O	O49	0.970279	0.744311	0.166137
O	O50	0.826510	0.829594	0.122028
O	O51	0.564466	0.924788	0.622321
O	O52	0.863600	0.878841	0.467143
O	O53	0.905969	0.596206	0.285325
O	O54	0.698154	0.937263	0.504670
O	O55	0.583963	0.714773	0.834622
O	O56	0.813437	0.859498	0.792428
O	O57	0.918820	0.727206	0.442476
O	O58	0.695916	0.628061	0.083004
O	O59	0.503751	0.880374	0.465125
O	O60	0.840079	0.933881	0.640056
O	O61	0.841033	0.542651	0.129681
O	O62	0.888949	0.827536	0.302198
O	O63	0.845976	0.501598	0.459754
O	O64	0.509134	0.842347	0.799314
O	O65	0.624861	0.760477	0.097585
O	O66	0.737296	0.985024	0.751407
O	O67	0.837668	0.446689	0.618354
O	O68	0.490886	0.163222	0.461394
O	O69	0.636767	0.078143	0.508769
O	O70	0.718413	0.307770	0.502673
O	O71	0.602700	0.431276	0.841806
O	O72	0.524347	0.204726	0.794783
O	O73	0.928942	0.107765	0.509535
O	O74	0.922921	0.378272	0.505091
O	O75	0.590202	0.072074	0.764060
O	O76	0.941492	0.061220	0.768413
O	O77	0.800566	0.501187	0.793694
O	O78	0.612923	0.394510	0.092158
O	O79	0.722814	0.275057	0.747260
O	O80	0.956611	0.426938	0.764952
O	O81	0.564536	0.178184	0.639275
O	O82	0.498335	0.775681	0.954221
O	O83	0.760451	0.523321	0.951465
O	O84	0.749566	0.779813	0.970067
O	O85	0.405220	0.968430	0.165302
O	O86	0.380239	0.643799	0.833356
O	O87	0.271529	0.764247	0.174826
O	O88	0.048668	0.977918	0.172198
O	O89	0.192444	0.534565	0.132378
O	O90	0.153377	0.530703	0.463393
O	O91	0.038259	0.608320	0.166366

O	O92	0.425598	0.856271	0.287149
O	O93	0.171605	0.594011	0.306852
O	O94	0.359718	0.964155	0.417960
O	O95	0.277885	0.730077	0.428421
O	O96	0.391211	0.606998	0.085455
O	O97	0.066416	0.935900	0.407112
O	O98	0.470902	0.835976	0.130700
O	O99	0.073034	0.650297	0.417625
O	O100	0.237410	0.252925	0.954021
O	O101	0.499035	0.258967	0.972548
O	O102	0.234328	0.517601	0.975097
O	O103	0.873010	0.717004	0.612513
Al	Al104	0.269602	0.287389	0.066557
Al	Al105	0.056626	0.186147	0.733858
Al	Al106	0.159567	0.074652	0.398036
Al	Al107	0.061896	0.416546	0.527444
Al	Al108	0.390754	0.082833	0.193616
Al	Al109	0.498649	0.292282	0.860879
Al	Al110	0.935953	0.621578	0.398864
Al	Al111	0.600022	0.955814	0.734401
Al	Al112	0.496622	0.745588	0.067817
Al	Al113	0.721356	0.747494	0.858371
Al	Al114	0.933407	0.846309	0.194593
Al	Al115	0.833987	0.964698	0.525754
Al	Al116	0.728586	0.522639	0.064980
Al	Al117	0.830144	0.413035	0.731439
Al	Al118	0.601419	0.181033	0.527367
Al	Al119	0.391358	0.858424	0.398890
Al	Al120	0.266645	0.515740	0.863363
Al	Al121	0.167485	0.625635	0.194700
Si	Si122	0.934857	0.845405	0.402539
P	P123	0.054449	0.185438	0.524638
P	P124	0.161314	0.079608	0.191698
P	P125	0.270090	0.288954	0.857601
P	P126	0.269270	0.515866	0.071571
P	P127	0.391269	0.086258	0.403017
P	P128	0.056634	0.416000	0.736964
P	P129	0.725146	0.521982	0.855034
P	P130	0.601070	0.955626	0.525256
P	P131	0.939100	0.624154	0.187502
P	P132	0.832625	0.960581	0.737717
P	P133	0.724827	0.749520	0.068782
P	P134	0.832160	0.408730	0.521540
P	P135	0.600890	0.182787	0.736101

P	P136	0.500601	0.293077	0.069811
P	P137	0.392962	0.856007	0.189674
P	P138	0.493125	0.744272	0.856257
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TS-Elimination-TMB-C3-H2O-Si-AlPO-34

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H	H3	0.506111	0.377696	0.646416
H	H4	0.598485	0.402851	0.555561
H	H5	0.525966	0.622051	0.238380
H	H6	0.650850	0.676720	0.298513
H	H7	0.570494	0.742572	0.304751
H	H8	0.599717	0.469660	0.300996
H	H9	0.473796	0.430532	0.246189
H	H10	0.481744	0.338662	0.323360
H	H11	0.572144	0.578555	0.660001
H	H12	0.433552	0.630052	0.659004
H	H13	0.299664	0.579989	0.616210
H	H14	0.408476	0.710723	0.582244
H	H15	0.315094	0.306218	0.601943
H	H16	0.374277	0.426674	0.669709
H	H17	0.248384	0.384887	0.615893
H	H18	0.766818	0.661629	0.590133
H	H19	0.696099	0.591329	0.487471
H	H20	0.672752	0.699642	0.534673
H	H21	0.892295	0.787705	0.635024

H	H22	0.397005	0.328342	0.461468
H	H23	0.492688	0.719690	0.444547
C	C24	0.587027	0.434986	0.617952
C	C25	0.565410	0.661550	0.301089
C	C26	0.475580	0.476815	0.383114
C	C27	0.509063	0.425768	0.309842
C	C28	0.418386	0.414891	0.457489
C	C29	0.389323	0.460543	0.528686
C	C30	0.604342	0.548419	0.607621
C	C31	0.415192	0.572393	0.523673
C	C32	0.387765	0.626213	0.598697
C	C33	0.470465	0.633326	0.448369
C	C34	0.502467	0.589252	0.378622
C	C35	0.329135	0.390624	0.608006
C	C36	0.674643	0.623370	0.545382
O	O37	0.076436	0.303729	0.504401
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O	O39	0.153132	0.491542	0.794080
O	O40	0.168392	0.121525	0.283970
O	O41	0.079613	0.173604	0.619288
O	O42	0.369878	0.277593	0.829905
O	O43	0.252760	0.049798	0.172409
O	O44	0.483276	0.198241	0.130272
O	O45	0.172459	0.212793	0.794343
O	O46	0.258748	0.403945	0.094191
O	O47	0.025804	0.293165	0.746519
O	O48	0.422912	0.114325	0.304321
O	O49	0.129543	0.165073	0.462247
O	O50	0.083137	0.451392	0.638941
O	O51	0.295328	0.108210	0.426222
O	O52	0.407790	0.321676	0.081844
O	O53	0.176714	0.172547	0.125392
O	O54	0.732635	0.631732	0.826134
O	O55	0.969522	0.743289	0.164602
O	O56	0.825224	0.828967	0.121590
O	O57	0.566136	0.924552	0.620091
O	O58	0.857549	0.873222	0.465383
O	O59	0.903348	0.595647	0.284524
O	O60	0.696614	0.937637	0.499259
O	O61	0.582382	0.715187	0.837162
O	O62	0.810796	0.857814	0.789259
O	O63	0.923821	0.730568	0.440811
O	O64	0.694316	0.627700	0.082651
O	O65	0.503291	0.890066	0.463343

O	O66	0.835773	0.933926	0.637594
O	O67	0.839907	0.541606	0.128929
O	O68	0.890605	0.828526	0.300777
O	O69	0.845942	0.505036	0.459904
O	O70	0.507614	0.841296	0.796068
O	O71	0.625141	0.762143	0.091699
O	O72	0.736630	0.985927	0.751741
O	O73	0.836248	0.446700	0.617843
O	O74	0.489036	0.158234	0.459823
O	O75	0.643075	0.083702	0.511351
O	O76	0.714275	0.311494	0.501008
O	O77	0.601609	0.429787	0.845994
O	O78	0.523034	0.204244	0.793623
O	O79	0.929361	0.103997	0.503978
O	O80	0.918186	0.377238	0.502755
O	O81	0.587477	0.070764	0.761676
O	O82	0.940645	0.059518	0.766105
O	O83	0.797689	0.499179	0.793006
O	O84	0.612263	0.394212	0.087734
O	O85	0.721024	0.273626	0.745422
O	O86	0.953869	0.424421	0.765476
O	O87	0.562035	0.178263	0.637884
O	O88	0.496415	0.780957	0.952885
O	O89	0.763822	0.528286	0.950632
O	O90	0.753645	0.778938	0.968031
O	O91	0.404668	0.968073	0.161875
O	O92	0.378666	0.644472	0.834467
O	O93	0.270301	0.764166	0.173318
O	O94	0.048398	0.977406	0.169327
O	O95	0.192787	0.535717	0.129602
O	O96	0.150454	0.529025	0.462473
O	O97	0.037069	0.606770	0.167222
O	O98	0.422523	0.858280	0.286936
O	O99	0.174676	0.593971	0.305612
O	O100	0.349286	0.960794	0.417159
O	O101	0.278376	0.728516	0.428990
O	O102	0.391017	0.607604	0.080759
O	O103	0.064684	0.941896	0.408331
O	O104	0.470583	0.834528	0.132386
O	O105	0.074120	0.650542	0.413673
O	O106	0.235970	0.256475	0.951320
O	O107	0.495854	0.253021	0.971915
O	O108	0.231691	0.512393	0.972924
O	O109	0.877417	0.715553	0.613324

Al	Al110	0.268944	0.287833	0.064141
Al	Al111	0.055410	0.184966	0.731609
Al	Al112	0.160025	0.079448	0.395948
Al	Al113	0.056946	0.415529	0.525902
Al	Al114	0.389976	0.081894	0.191921
Al	Al115	0.497017	0.290273	0.861089
Al	Al116	0.937301	0.623174	0.397472
Al	Al117	0.599404	0.955595	0.732461
Al	Al118	0.495906	0.747048	0.065402
Al	Al119	0.720347	0.746854	0.856787
Al	Al120	0.933505	0.846060	0.192909
Al	Al121	0.831320	0.962392	0.522598
Al	Al122	0.728430	0.523267	0.063672
Al	Al123	0.828370	0.411842	0.730692
Al	Al124	0.600919	0.182144	0.526432
Al	Al125	0.387185	0.859212	0.398581
Al	Al126	0.265194	0.514908	0.860893
Al	Al127	0.167353	0.625094	0.193855
Si	Si128	0.934880	0.846595	0.401751
P	P129	0.053275	0.185548	0.521932
P	P130	0.160810	0.079436	0.188824
P	P131	0.269352	0.289637	0.854525
P	P132	0.268923	0.515346	0.069374
P	P133	0.388025	0.084628	0.401620
P	P134	0.054111	0.414654	0.735883
P	P135	0.724134	0.521858	0.854971
P	P136	0.602670	0.959341	0.523531
P	P137	0.937893	0.623168	0.186908
P	P138	0.830652	0.960027	0.735691
P	P139	0.725142	0.749551	0.066493
P	P140	0.829529	0.410260	0.520462
P	P141	0.598850	0.181936	0.734428
P	P142	0.499581	0.291852	0.068031
P	P143	0.391558	0.855932	0.188792
P	P144	0.491533	0.745597	0.855971
P	P145	0.168871	0.625421	0.402256