SUPPORTING INFORMATION

Assessment of the Behaviour of Two Host Systems in the Presence of Single and Mixed Isomers of Cyclohexanone and MethylCyclohexanones

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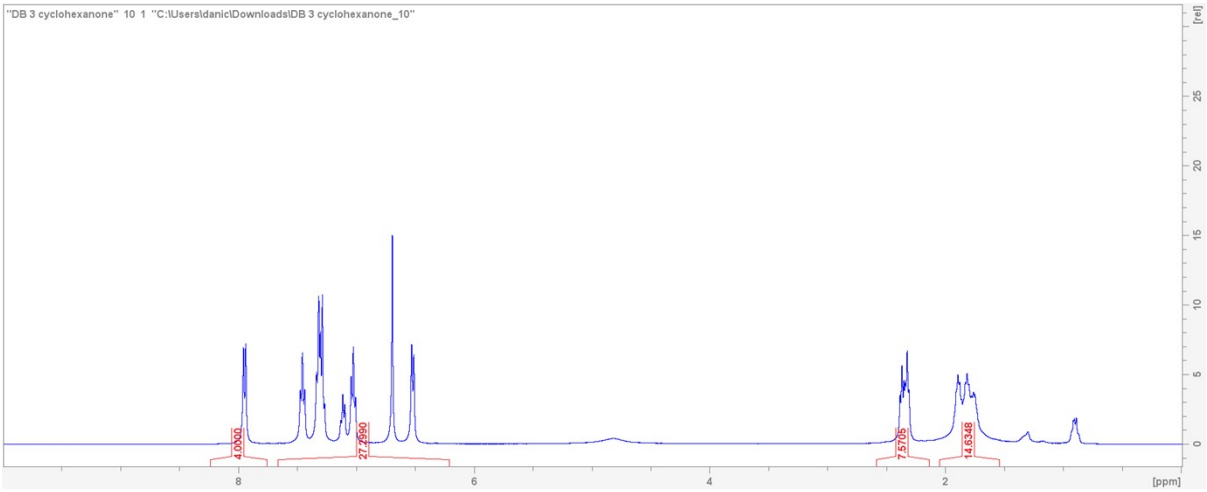
a)



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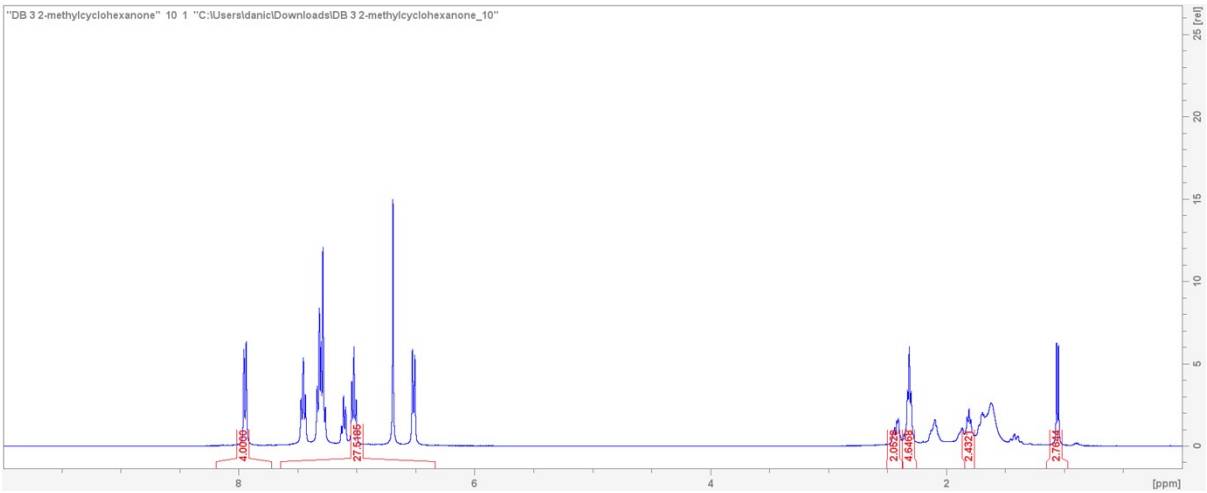

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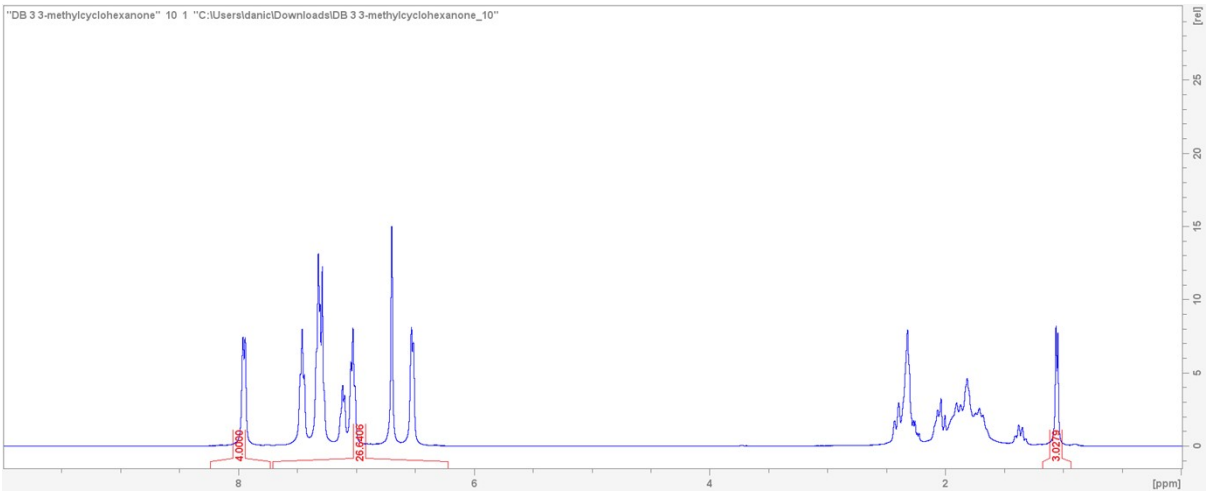

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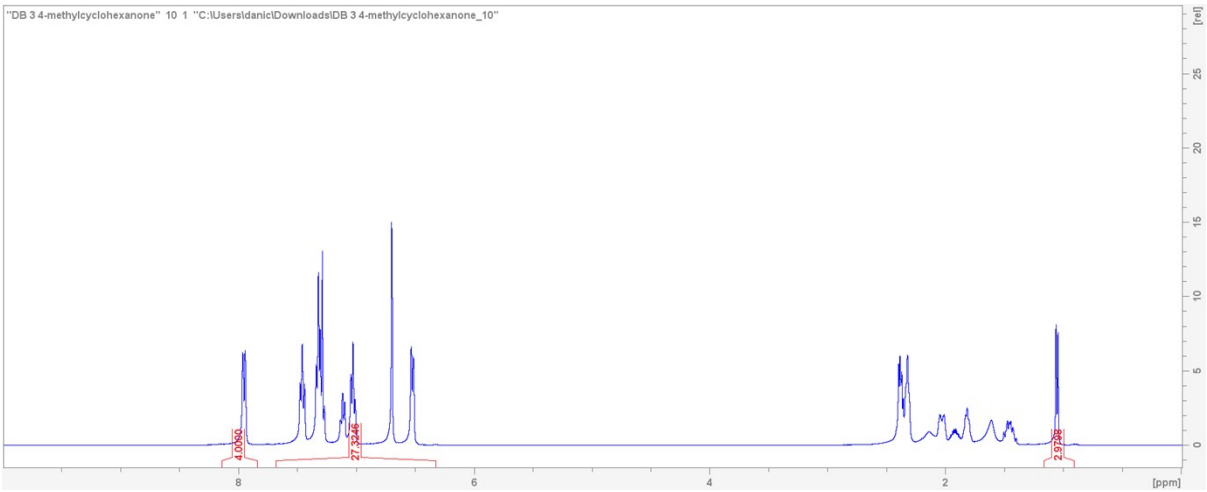

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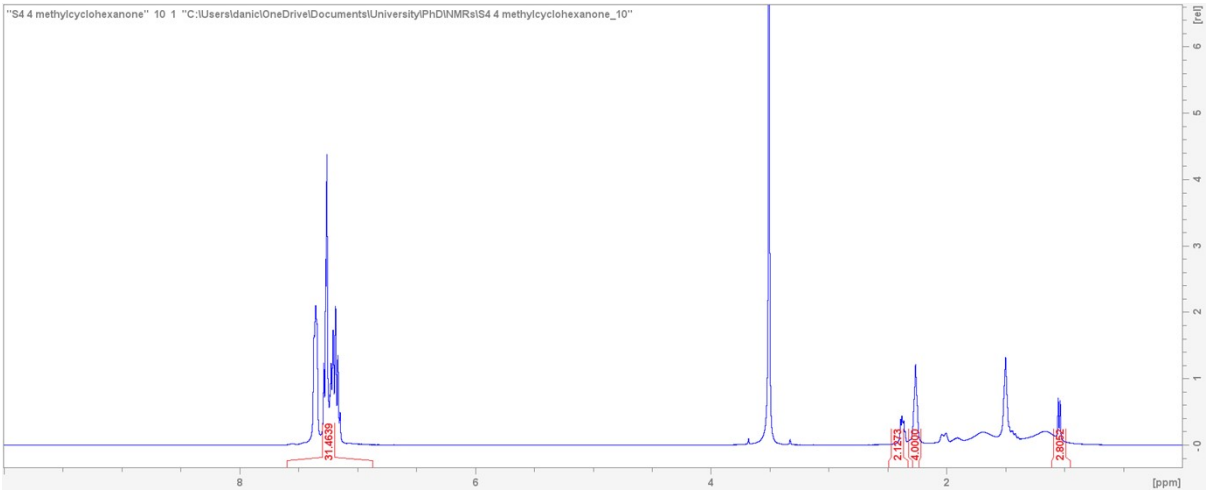


Figure S1 ^{1}H-NMR spectra for a) **DB3**·Cyc, b) **DB3**·2MeCyc, c) **DB3**·3MeCyc, d) **DB3**·4MeCyc, and e) **S4**·4MeCyc.

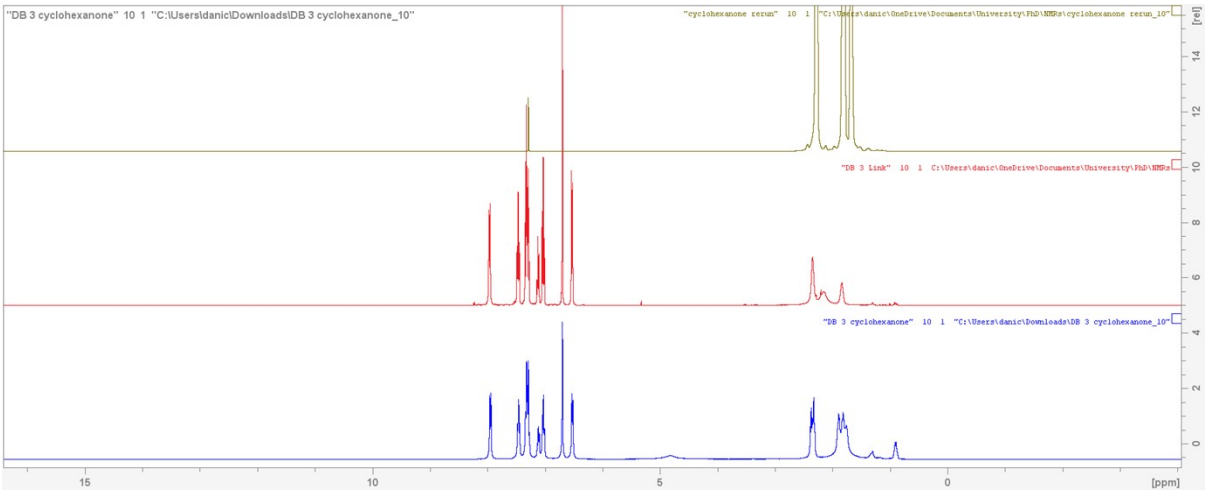


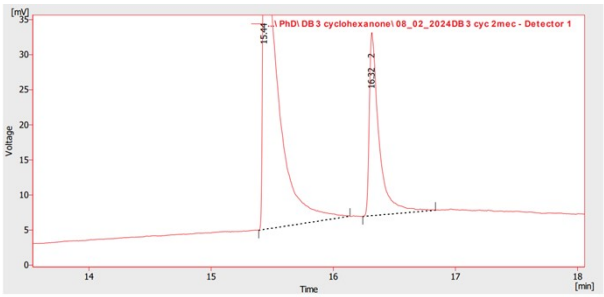
Figure S2 Stacked ^{1}H-NMR spectra for **DB3**·Cyc (blue), **DB3** host alone (red) and Cyc (olive green).

Table S1 G:G percentages and *K* values obtained in the various molar concentrations of binary guests involving **DB3**.

Cyc/2MeCyc			Cyc/3MeCyc			Cyc/4MeCyc			2MeCyc/3MeCyc			2MeCyc/4MeCyc			3MeCyc/4MeCyc		
Molar conc) of Cyc	G_A:G_B	*K*	Molar conc) of Cyc	G_A:G_B	*K*	Molar conc) of 4MeCyc	G_A:G_B	*K*	Molar conc) of 2MeCyc	G_A:G_B	*K*	Molar conc) of 4MeCyc	G_A:G_B	*K*	Molar conc) of 4MeCyc	G_A:G_B	*K*
80	90.6	2.4	80	94	3.9	20[a]	16	1.3	80	84.1	1.3	20	26.1	1.4	20	29.5	1.7
60	77.7	2.3	60	85.5	3.9	40[a]	33.9	1.3	60	64.9	1.2	40	49.0	1.4	40	55.7	1.9
50	71.2	2.5	50	76.4	3.2	50	57.55	1.4	50[a]	47.1	1.1	50	58.9	1.4	50	67.7	2.1
40	43.8	1.2	40	69.7	3.5	60	62.3	1.1	40	43.7	1.2	60	69.3	1.5	60	76.0	2.1
20[a]	9.0	2.5	20[a]	9.8	2.3	80	92.6	3.1	20	21.1	1.1	80	86.8	1.6	80	89.7	2.2

[a]The *K* value is calculated in favour of the other guest present and not the most preferred guest solvent.

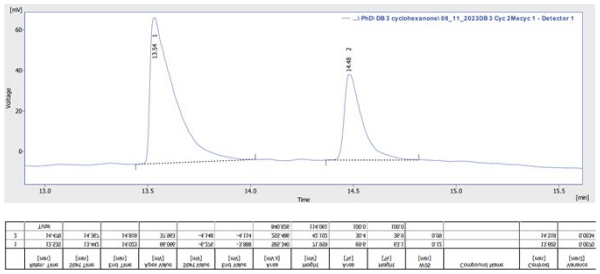
a)



Result Table (Uncal - C:\Clarity\DataFiles\Danica\Data\PhD\DB 3 cyclohexanone\08_02_2024DB 3 cyc 2mec - Detector 1)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]	Compound Name
1	15.435	389.927	47.249	72.8	64.4	0.11	
2	16.315	145.747	26.105	27.2	35.6	0.07	
	Total	535.674	73.355	100.0	100.0		

b)



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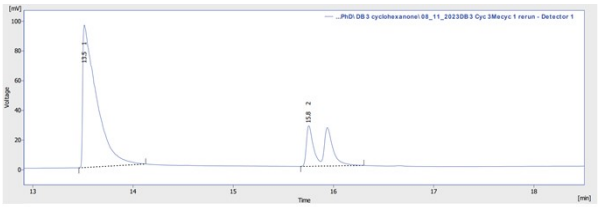

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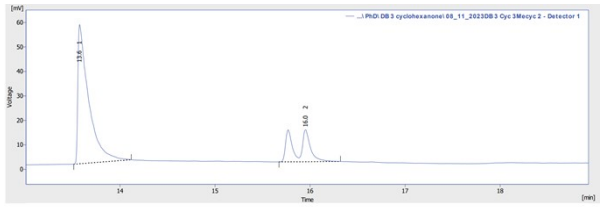

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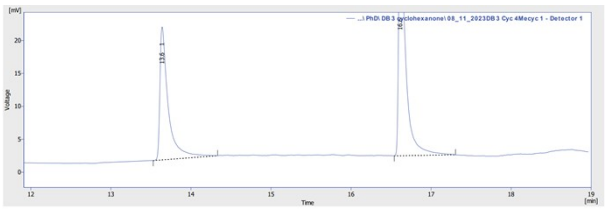

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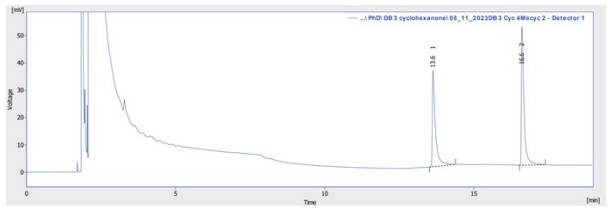

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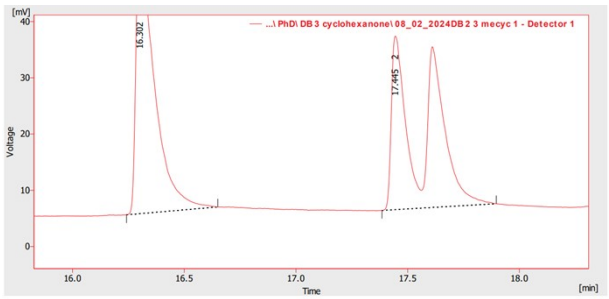
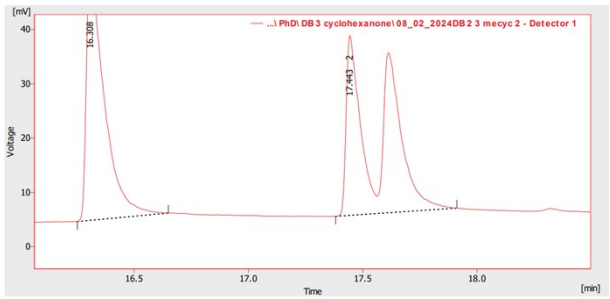


Result Table (Uncal - C:\Clarity\DataFiles\Danica\Data\PhD\DB 3 cyclohexanone\08_02_2024DB 2 3 mecyc 1 - Detector 1)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]	Compound Name
1	16.302	277.523	48.992	48.9	61.4	0.08	
2	17.445	289.856	30.861	51.1	38.6	0.07	
	Total	567.378	79.853	100.0	100.0		

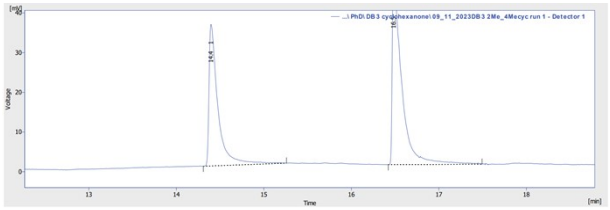
h)



Result Table (Uncal - C:\Clarity\DataFiles\Danica\Data\PhD\DB 3 cyclohexanone\08_02_2024DB 2 3 mecyc 2 - Detector 1)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]	Compound Name
1	16.308	252.139	45.460	45.3	57.9	0.08	
2	17.443	305.050	33.099	54.7	42.1	0.07	
	Total	557.189	78.559	100.0	100.0		

i)



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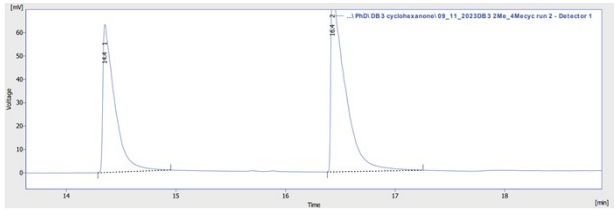

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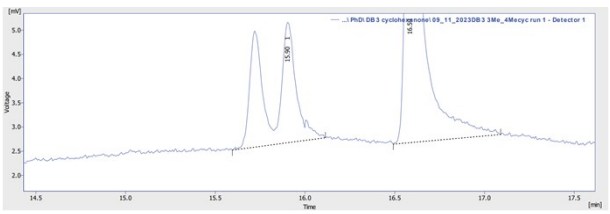

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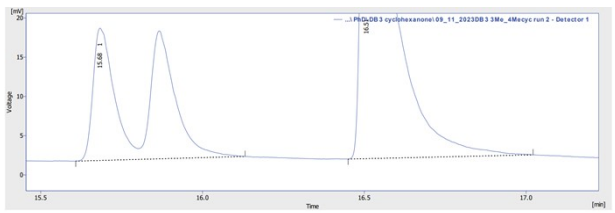


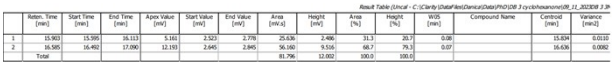


Figure S3 Host compounds **DB3** with the duplicate GC data for CYC/2MECYC in a) and b), for Cyc/3MeCyc in c) and d), for Cyc/4MeCyc in e) and f), for 2MeCyc/4MeCyc in g) and h), and for 3MeCyc/4MeCyc in i) and j).

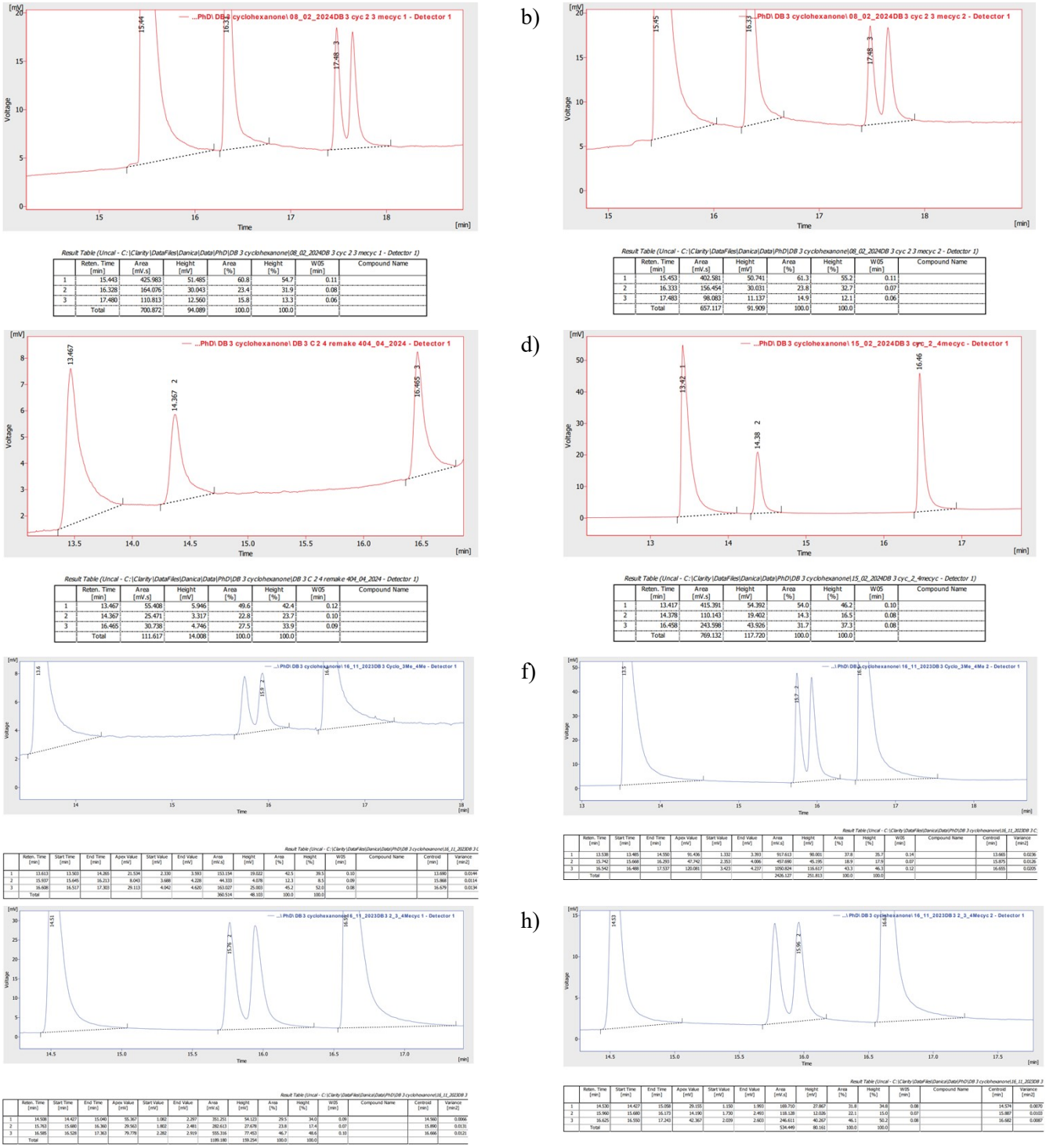
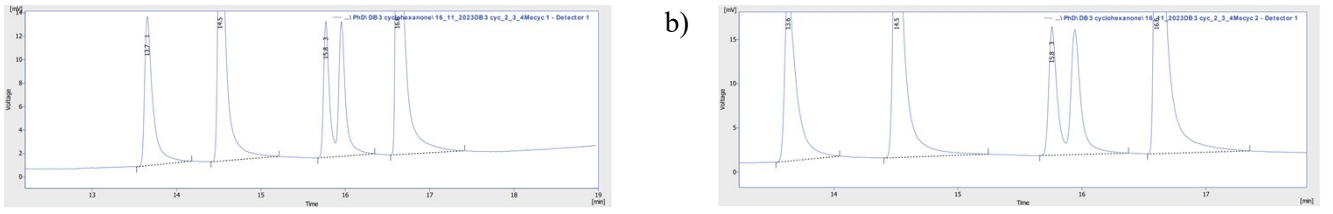
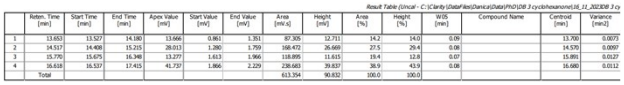


Figure S4 Host compounds **DB3** GC data with Cyc/2MeCyc/3MeCyc in a) and b), with Cyc/2MeCyc/4MeCyc in c) and d), with Cyc/3MeCyc/4MeCyc in e) and f), and with 2MeCyc/3MeCyc/4MeCyc in g) and h).





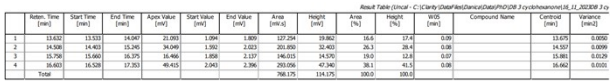
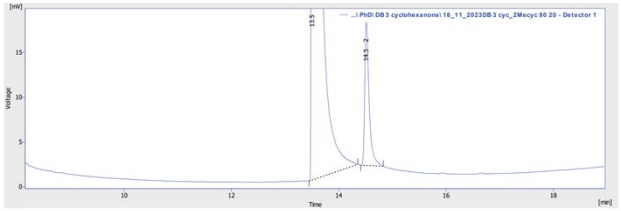
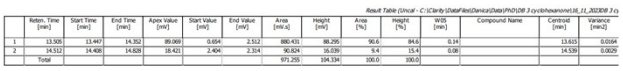


Figure S5 Host compounds **DB3** GC data with all four Cyc/MeCyc's in a) and b).

a)





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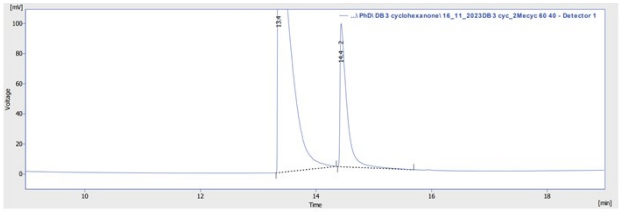

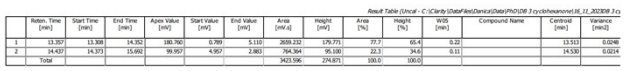

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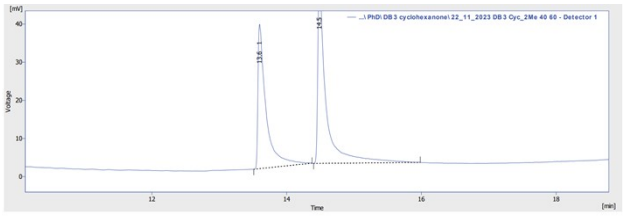

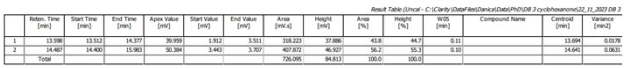

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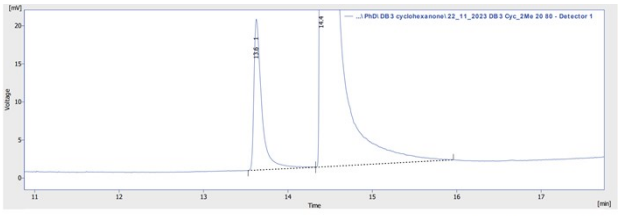


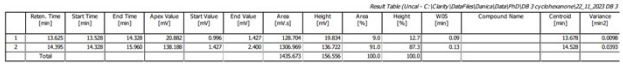
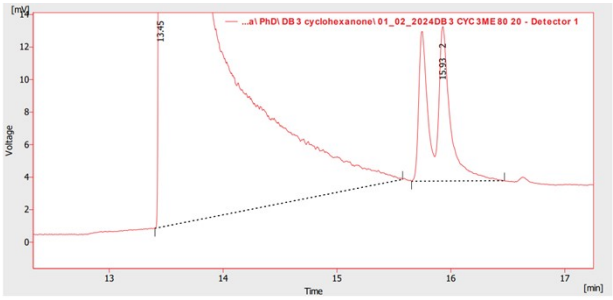


Figure S6 Host compounds **DB3** for the selectivity profile Cyc/2MeCyc for the crystals with a) 80 20, b) 60 40, c) 40 60, and d) 20 80 concentrations.

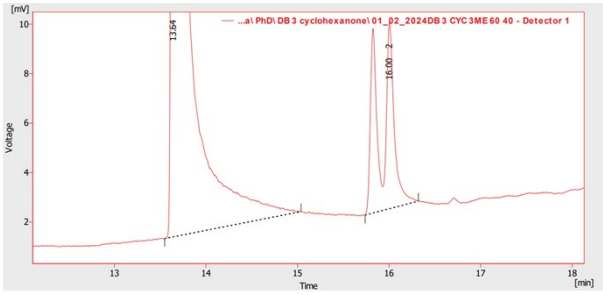
a)



Result Table (Uncal - C:\Clarity\DataFiles\Danica\Data\PhD\DB 3 cyclohexanone\01_02_2024DB 3 CYC 3ME 80 20 - Detector 1)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]	Compound Name
1	13.453	1804.737	115.874	94.0	92.4	0.17	
2	15.930	114.857	9.498	6.0	7.6	0.09	
	Total	1919.594	125.372	100.0	100.0		

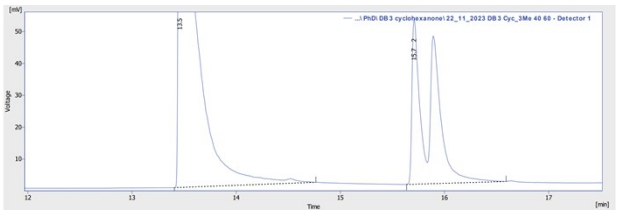
b)

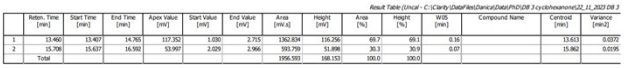


Result Table (Uncal - C:\Clarity\DataFiles\Danica\Data\PhD\DB 3 cyclohexanone\01_02_2024DB 3 CYC 3ME 60 40 - Detector 1)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]	Compound Name
1	13.643	475.176	51.281	85.5	87.2	0.11	
2	16.003	80.496	7.533	14.5	12.8	0.08	
	Total	555.672	58.814	100.0	100.0		

c)





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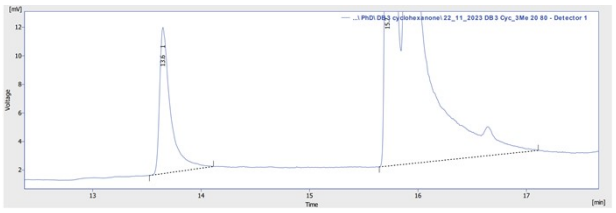


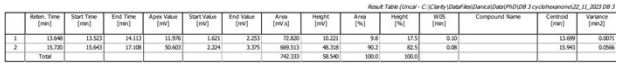
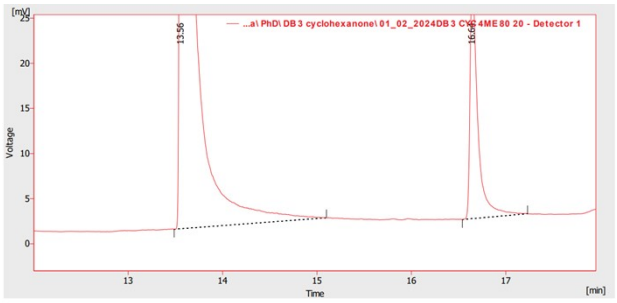


Figure S7 Host compounds **DB3** for the selectivity profile Cyc/3MeCyc for the crystals with a) 80 20, b) 60 40, c) 40 60, and d) 20 80 concentrations.

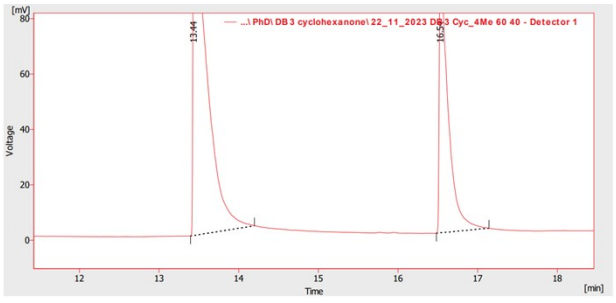
a)



Result Table (Uncal - C:\Clarity\DataFiles\Danica\Data\PhD\DB 3 cyclohexanone\01_02_2024DB 3 CYC 4ME 80 20 - Detector 1)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]	Compound Name
1	13.557	796.907	78.393	84.0	74.5	0.13	
2	16.643	151.794	26.844	16.0	25.5	0.07	
	Total	948.701	105.236	100.0	100.0		

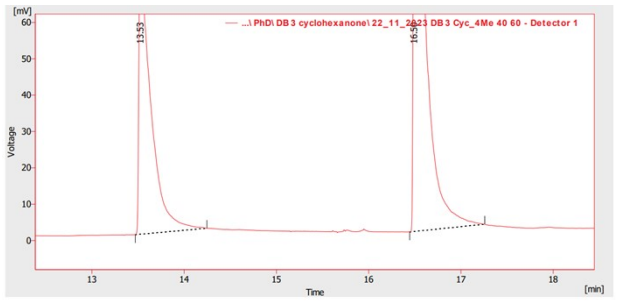
b)



Result Table (Uncal - C:\Clarity\DataFiles\Danica\Data\PhD\DB 3 cyclohexanone\22_11_2023 DB 3 Cyc_4Me 60 40 - Detector 1)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]	Compound Name
1	13.438	1465.428	125.219	66.1	55.7	0.17	
2	16.535	752.928	99.578	33.9	44.3	0.11	
	Total	2218.356	224.797	100.0	100.0		

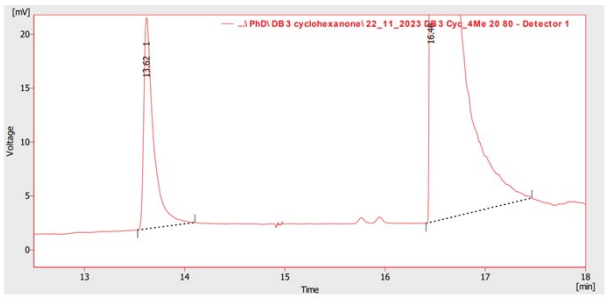
c)



Result Table (Uncal - C:\Clarity\DataFiles\Danica\Data\PhD\DB 3 cyclohexanone\22_11_2023 DB 3 Cyc_4Me 40 60 - Detector 1)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]	Compound Name
1	13.527	690.857	78.030	37.7	37.9	0.12	
2	16.495	1142.364	127.812	62.3	62.1	0.13	
	Total	1833.220	205.842	100.0	100.0		

d)



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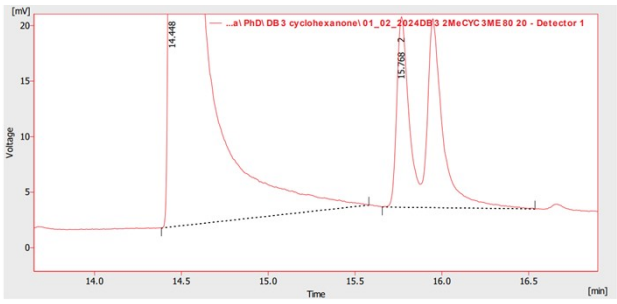
	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]	Compound Name
1	13.620	133.330	19.592	7.4	11.2	0.09	
2	16.460	1666.996	155.592	92.6	88.8	0.14	
	Total	1800.326	175.184	100.0	100.0		

Figure S8 Host compounds **DB3** for the selectivity profile Cyc/4MeCyc for the crystals with a) 80 20, b) 60 40, c) 40 60, and d) 20 80 concentrations.

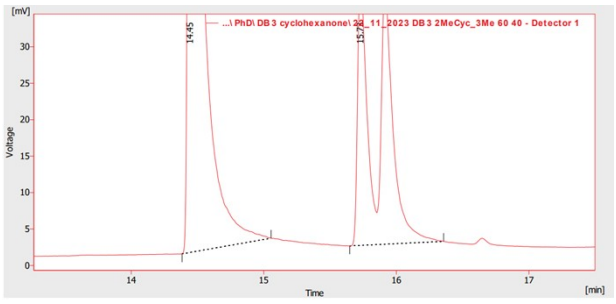
a)



Result Table (Uncal - C:\Clarity\DataFiles\Danica\Data\PhD\DB 3 cyclohexanone\01_02_2024DB 3 2MeCYC 3ME 80 20 - Detector 1)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]	Compound Name
1	14.448	990.733	113.959	84.1	86.9	0.11	
2	15.768	186.881	17.135	15.9	13.1	0.07	
	Total	1177.614	131.094	100.0	100.0		

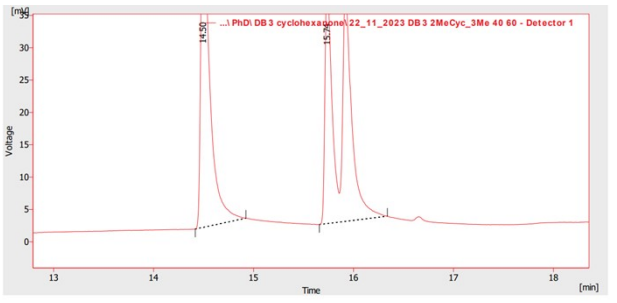
b)



Result Table (Uncal - C:\Clarity\DataFiles\Danica\Data\PhD\DB 3 cyclohexanone\22_11_2023 DB 3 2MeCyc_3Me 60 40 - Detector 1)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]	Compound Name
1	14.445	742.511	98.599	64.9	72.8	0.11	
2	15.730	402.010	36.920	35.1	27.2	0.07	
	Total	1144.521	135.519	100.0	100.0		

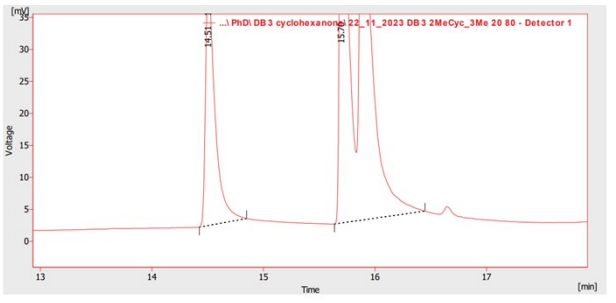
c)



Result Table (Uncal - C:\Clarity\DataFiles\Danica\Data\PhD\DB 3 cyclohexanone\22_11_2023 DB 3 2MeCyc_3Me 40 60 - Detector 1)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]	Compound Name
1	14.497	316.697	50.852	43.7	57.6	0.09	
2	15.738	408.566	37.487	56.3	42.4	0.07	
	Total	725.263	88.338	100.0	100.0		

d)

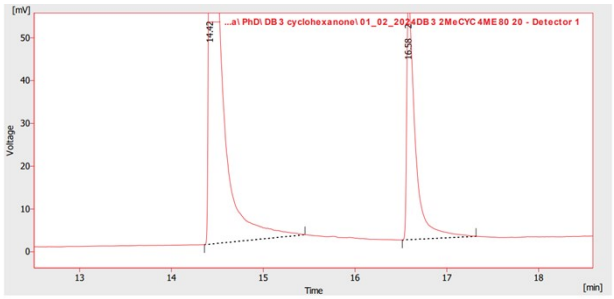


Result Table (Uncal - C:\Clarity\DataFiles\Danica\Data\PhD\DB 3 cyclohexanone\22_11_2023 DB 3 2MeCyc_3Me 20 80 - Detector 1)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]	Compound Name
1	14.507	226.479	37.812	21.1	35.3	0.09	
2	15.700	849.273	69.249	78.9	64.7	0.08	
	Total	1075.752	107.061	100.0	100.0		

Figure S9 Host compounds **DB3** for the selectivity profile 2MeCyc/3MeCyc for the crystals with a) 80 20, b) 60 40, c) 40 60, and d) 20 80 concentrations.

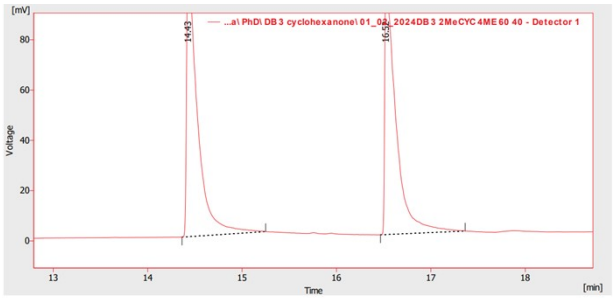
a)



Result Table (Uncal - C:\Clarity\DataFiles\Danica\Data\PhD\DB 3 cyclohexanone\01_02_2024DB 3 2MeCYC 4ME 80 20 - Detector 1)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]	Compound Name
1	14.422	1038.235	121.530	73.9	68.1	0.11	
2	16.583	367.069	57.011	26.1	31.9	0.09	
	Total	1405.304	178.541	100.0	100.0		

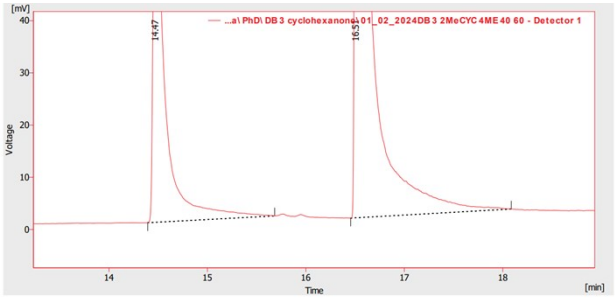
b)



Result Table (Uncal - C:\Clarity\DataFiles\Danica\Data\PhD\DB 3 cyclohexanone\01_02_2024DB 3 2MeCYC 4ME 60 40 - Detector 1)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]	Compound Name
1	14.430	873.966	109.363	51.0	51.1	0.11	
2	16.525	838.421	104.813	49.0	48.9	0.11	
	Total	1712.387	214.176	100.0	100.0		

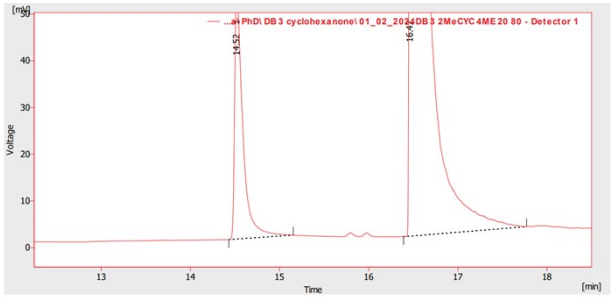
c)



Result Table (Uncal - C:\Clarity\DataFiles\Danica\Data\PhD\DB 3 cyclohexanone\01_02_2024DB 3 2MeCYC 4ME 40 60 - Detector 1)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]	Compound Name
1	14.472	593.353	71.719	30.7	36.2	0.10	
2	16.508	1338.173	126.608	69.3	63.8	0.12	
	Total	1931.526	198.326	100.0	100.0		

d)

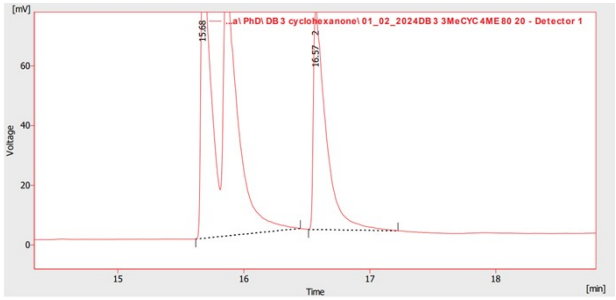


Result Table (Uncal - C:\Clarity\DataFiles\Danica\Data\PhD\DB 3 cyclohexanone\01_02_2024DB 3 2MeCYC 4ME 20 80 - Detector 1)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]	Compound Name
1	14.520	339.269	53.076	13.2	21.9	0.09	
2	16.465	2237.101	189.675	86.8	78.1	0.16	
	Total	2576.370	242.751	100.0	100.0		

Figure S10 Host compounds **DB3** for the selectivity profile 2MeCyc/4MeCyc for the crystals with a) 80 20, b) 60 40, c) 40 60, and d) 20 80 concentrations.

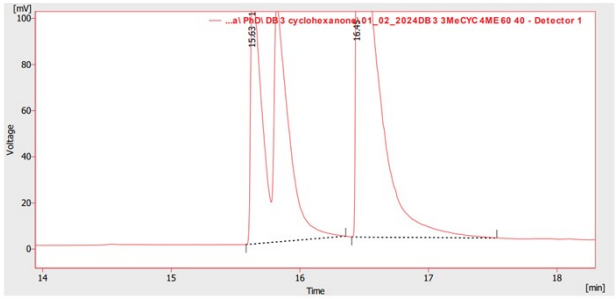
a)



Result Table (Uncal - C:\Clarity\DataFiles\Danica\Data\PhD\DB 3 cyclohexanone\01_02_2024DB 3 3MeCYC 4ME 80 20 - Detector 1)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]	Compound Name
1	15.675	1231.014	96.945	70.5	56.3	0.09	
2	16.572	515.761	75.288	29.5	43.7	0.10	
	Total	1746.775	172.234	100.0	100.0		

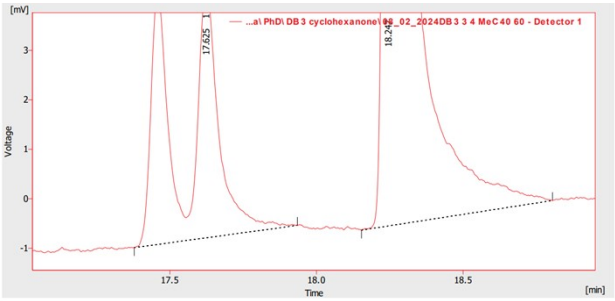
b)



Result Table (Uncal - C:\Clarity\DataFiles\Danica\Data\PhD\DB 3 cyclohexanone\01_02_2024DB 3 3MeCYC 4ME 60 40 - Detector 1)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]	Compound Name
1	15.632	1467.524	113.968	44.3	39.9	0.09	
2	16.447	1843.117	171.763	55.7	60.1	0.15	
	Total	3310.641	285.731	100.0	100.0		

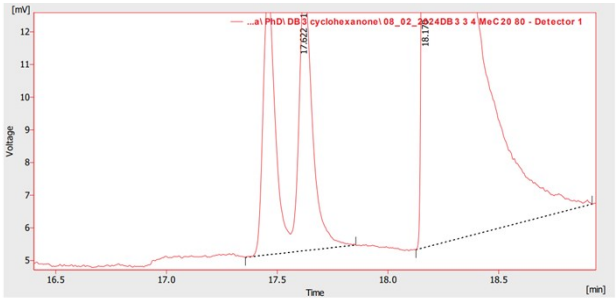
c)



Result Table (Uncal - C:\Clarity\DataFiles\Danica\Data\PhD\DB 3 cyclohexanone\08_02_2024DB 3 3 4 MeC 40 60 - Detector 1)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]	Compound Name
1	17.625	45.835	5.132	24.0	16.2	0.07	
2	18.247	145.022	26.501	76.0	83.8	0.07	
	Total	190.857	31.633	100.0	100.0		

d)



Result Table (Uncal - C:\Clarity\DataFiles\Danica\Data\PhD\DB 3 cyclohexanone\08_02_2024DB 3 3 4 MeC 20 80 - Detector 1)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]	Compound Name
1	17.622	65.876	8.221	10.3	10.3	0.06	
2	18.170	573.936	71.282	89.7	89.7	0.11	
	Total	639.812	79.503	100.0	100.0		

Figure S11 Host compounds **DB3** for the selectivity profile 3MeCyc/4MeCyc for the crystals with a) 80 20, b) 60 40, c) 40 60, and d) 20 80 concentrations.