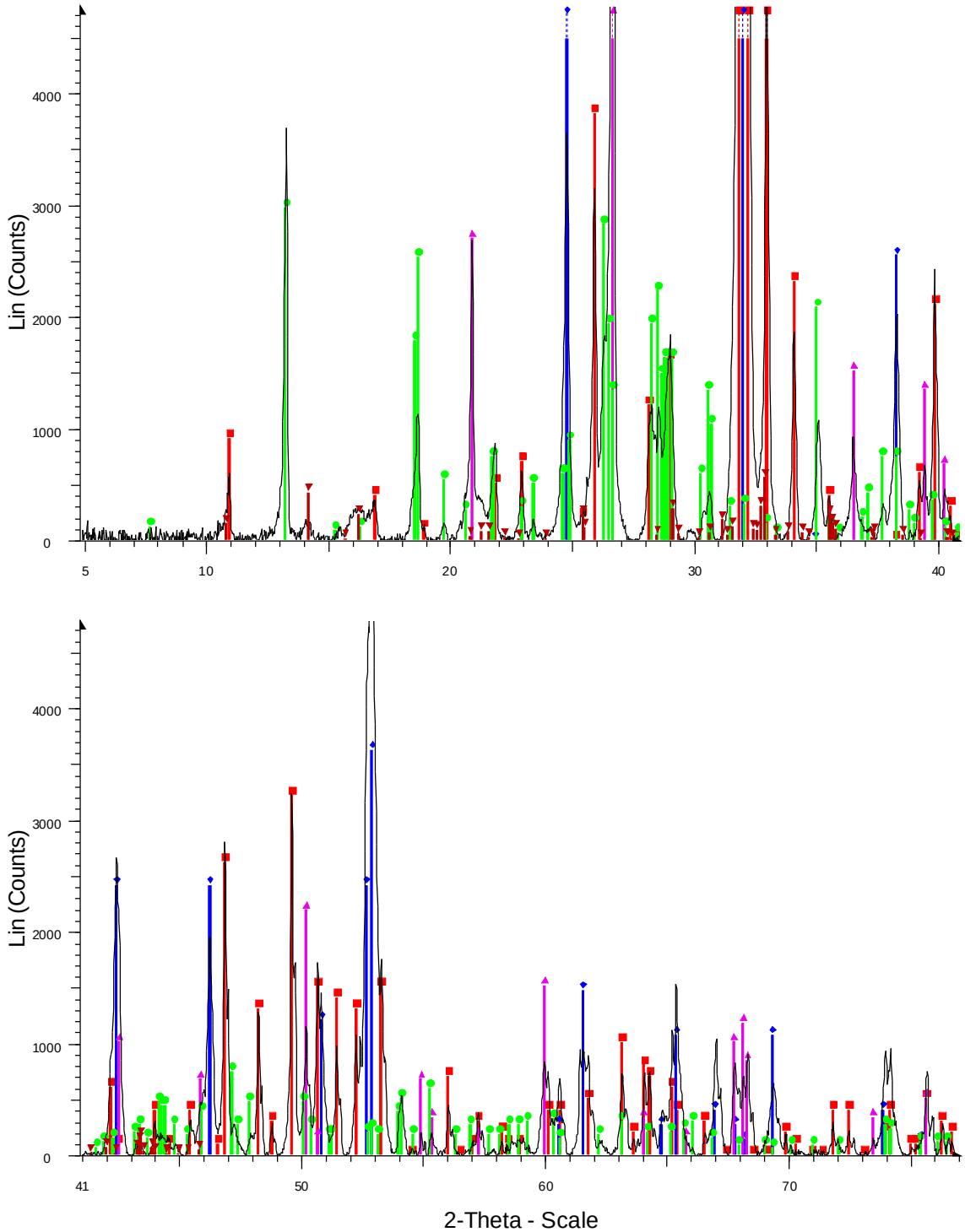
DiffracPlus Eva - SMRR1



SMRR-1 - File: smrr-1.raw - Type: 2Th/Th unlocked - Start: 4.840 ° - End: 76.874 ° - Step: 0.020 ° - Step time: 15. s - Temp.: 25 °C (Roo
Operations: Displacement 0.281 | Background 1.000,1.000 | Import

84-1997 (C) - Fluorapatite - Ca5(PO4)3F.94Cl.1 - Hexagonal - Y: 17.72 %

83-1764 (C) - Siderite - Fe(CO3) - Hexagonal (Rh) - Y: 23.63 %

46-1045 (*) - Quartz, syn - SiO2 - Hexagonal - Y: 29.70 %

36-0403 (I) - Gormanite - Fe3+2Al4(PO4)4(OH)6·2H2O - Triclinic - Y: 5.24 %

42-0581 (C) - Alluaudite - NaMn+2Fe2(PO4)3 - Monoclinic - Y: 0.98 %

Search results on SMRR-1 before correction of the sample displacement error:

Search performed on all Experimental & Inorganic patterns (62,016 patterns).
Good answers from this first run are in bold characters.

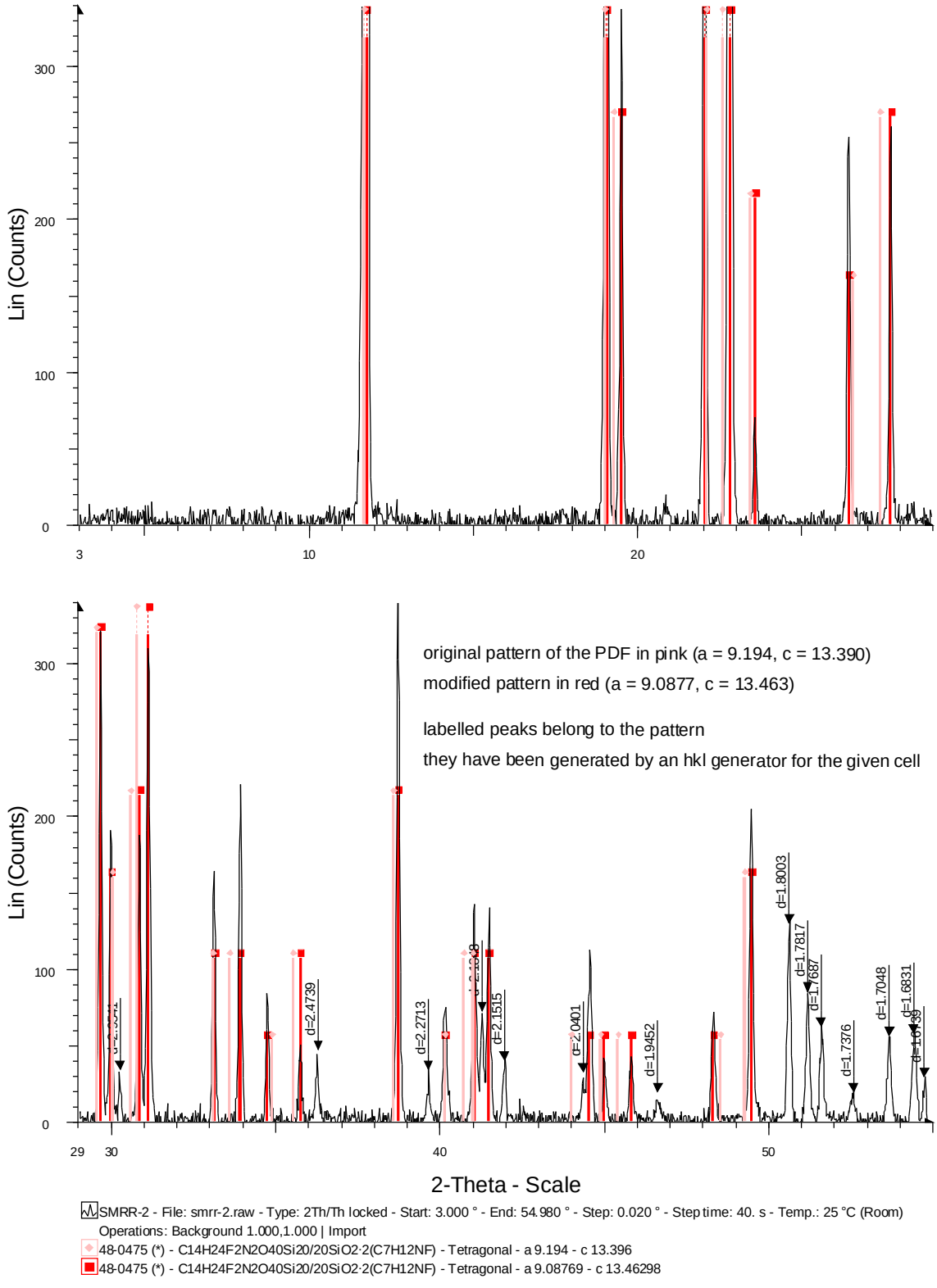
Scan: SMRR-1 (smrr-1.raw)
d multiplied by: 1.
2-theta offset: 0.000
Displacement: 0.
Criterion 3: Favor Complex Patterns
Databases: D:\PDF\PDF12-51\JCP2.CAT
Total Number: 136895
Match Chem./Subfile: 62016
Matching Intensity: 61916
Elapsed Time: 4.4

SS-NNNN	Compound Name	Formula	Mtc	nM	FOM	N°
32-0163 (*)		Ca8Gd2(PO4)6O2	41	11	1.9	1
48-1220 (*)		RbNiBr3·6H2O	59	17	1.91	2
15-0876 (*)	**Fluorapatite, syn**	**Ca5(PO4)3F**	**36**	**3**	**2.16**	**3**
48-1625 (*)		Y5Si3O12N	44	10	2.3	4
38-0256 (N)		Ca8Tb2(PO4)6O2	21	2	2.41	5
50-0493 (I)		Pb4BiVO8	26	6	2.43	6
44-0607 (C)		Mg15V6Mo6O48	79	31	2.81	7
29-0386 (I)		Ca2Tb8(SiO4)6O2	33	7	2.9	8
12-0531 (D)	**Siderite**	**FeCO3**	**12**	**0**	**3.23**	**9**
32-0557 (*)		LiGd9(SiO4)6O2	33	5	3.25	10
47-0744 (Q)		LiMnGa(MoO4)3	36	21	3.29	11
51-1854 (*)		K5Cd0.5Hf1.5(MoO4)6	75	40	3.37	12
41-1286 (C)		MnP4	75	53	3.43	13
21-0174 (D)	Britholite-(Y), syn	Ca2Y3Si3O12(OH)	20	1	3.45	14
44-1026 (I)		Cs3YbF6	37	8	3.51	15

Comments:

The trace is displayed after sample displacement error correction. The latter is 0.261 mm if we assume a diffractometer radius of 200 mm.

DiffracPlus Eva - SMRR-2



SMRR-2 - File: smrr-2.raw - Type: 2Th/Th locked - Start: 3.000 ° - End: 54.980 ° - Step: 0.020 ° - Step time: 40. s - Temp.: 25 °C (Room)
Operations: Background 1.000,1.000 | Import
48-0475 (*) - C14H24F2N2O40Si20/20SiO2·2(C7H12NF) - Tetragonal - a 9.194 - c 13.396
48-0475 (*) - C14H24F2N2O40Si20/20SiO2·2(C7H12NF) - Tetragonal - a 9.08769 - c 13.46298

Search results on SMRR-2:

Search performed on all Experimental patterns (85,381 patterns).
The one good answer from this first run is in bold characters.

Scan: SMRR-2 (smrr-2.raw)
d multiplied by: 1.
2-theta offset: 0.000
Displacement: 0.
Criterion 3: Favor Complex Patterns
Databases: D:\PDF\PDF12-51\JCP2.CAT
Total Number: 136895
Match Chem./Subfile: 85381
Matching Intensity: 82780
Elapsed Time: 4.

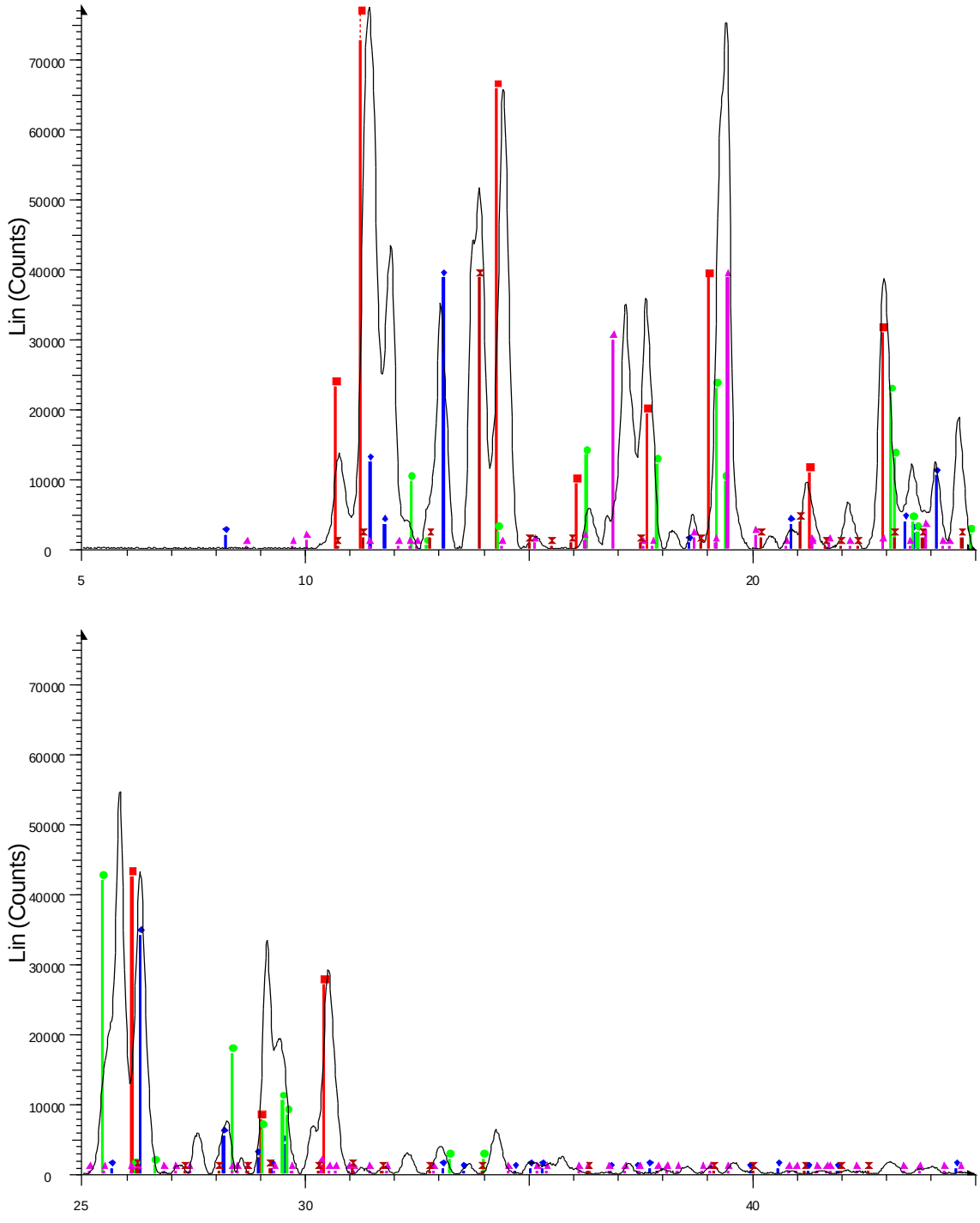
SS-NNNN	Compound Name	Formula	Mtc	nM	FOM	N°
44-1779 (*)		C7H8AsNO5	14	12	3.99	1
42-1678 (*)		(CH3)3NCH2COO·H3BO3	16	9	4.34	2
49-1267 (I)		C8H0.5K3.5O18Ti2·5.5H2O	21	20	4.39	3
42-1935 (I)		C8H24Cl6N2Zr/(N(CH3)4)2ZrCl6	11	6	6.07	4
12-0212 (D)	Graphite	C	4	1	6.44	5
50-2432 (*)		C6H8N4O4/C6H7N3O·HNO3	35	65	6.6	6
38-1007 (D)		PbBiO2I	10	3	6.67	7
43-1762 (I)		C15H15N3O4	26	18	7.37	8
34-0756 (Q)		K2Cr2O7	10	9	7.46	9
48-0475 (*)		**C14H24F2N2O40Si20/20SiO2·2(C7H12NF)**	**12**	**13**	**8.07**	**10**
51-0502 (N)		Sr2TmRuO6	8	13	8.46	11
30-0604 (D)		Au9In4	5	7	8.51	12
08-0415 (D)	Graphite	C	3	1	8.6	13
30-1794 (Q)		C14H12N2O	11	13	8.65	14
48-2430 (I)		C15H10N2O3	13	18	9.01	15

Comments:

There is a function in the Eva software that makes it possible to graphically adjust the cell parameters in order to try and get the best possible match with the unknown. The a parameter has been adjusted on the {200} line and the c parameter on the {004} one.

As the chemist told me that the phase could be a single phase, I have used an hkl-generator in order to check whether the residual lines (labelled on the plot) are explained by the found pattern. They are.

DiffracPlus Eva - SMRR3



SMRR-3 - File: smrr-3.raw - Type: 2Th/Th unlocked - Start: 5.000 ° - End: 45.000 ° - Step: 0.020 ° - Step time: 27. s - Temp.: 25 °C (Roo
Operations: Background 67.608,1.000 | Import

19-1946 (N) - Thalidomide - C13H10N2O - Monoclinic - Y: 100.00 %

45-1544 (*) - 6-Amino-phenalenone 6-amino-1H-phenalen-1-one - C13H9NO - Orthorhombic - Y: 50.00 %

48-2330 (Q) - N-Butyl-p-nitroaniline nona(p-nitroaniline) - C10H14N2O2·9(C6H6N2O2)/CH3(CH2)3NHC6H4NO2·9(H2NC6H4NO2) - Y: 54

47-2262 (I) - Tri(benzimidazolyl)amine hydrate - C24H21N7·H2O/(C6H4NNHCCH2)3N·H2O - Monoclinic - Y: 50.00 %

30-1806 (Q) - Methyl diphenyl-o-tolylacetate - C22H20O2 - Y: 50.00 %

Search results on SMRR-3:

Search performed on all Organic patterns (23,709 patterns).
The selected answers are from this run (in bold characters).

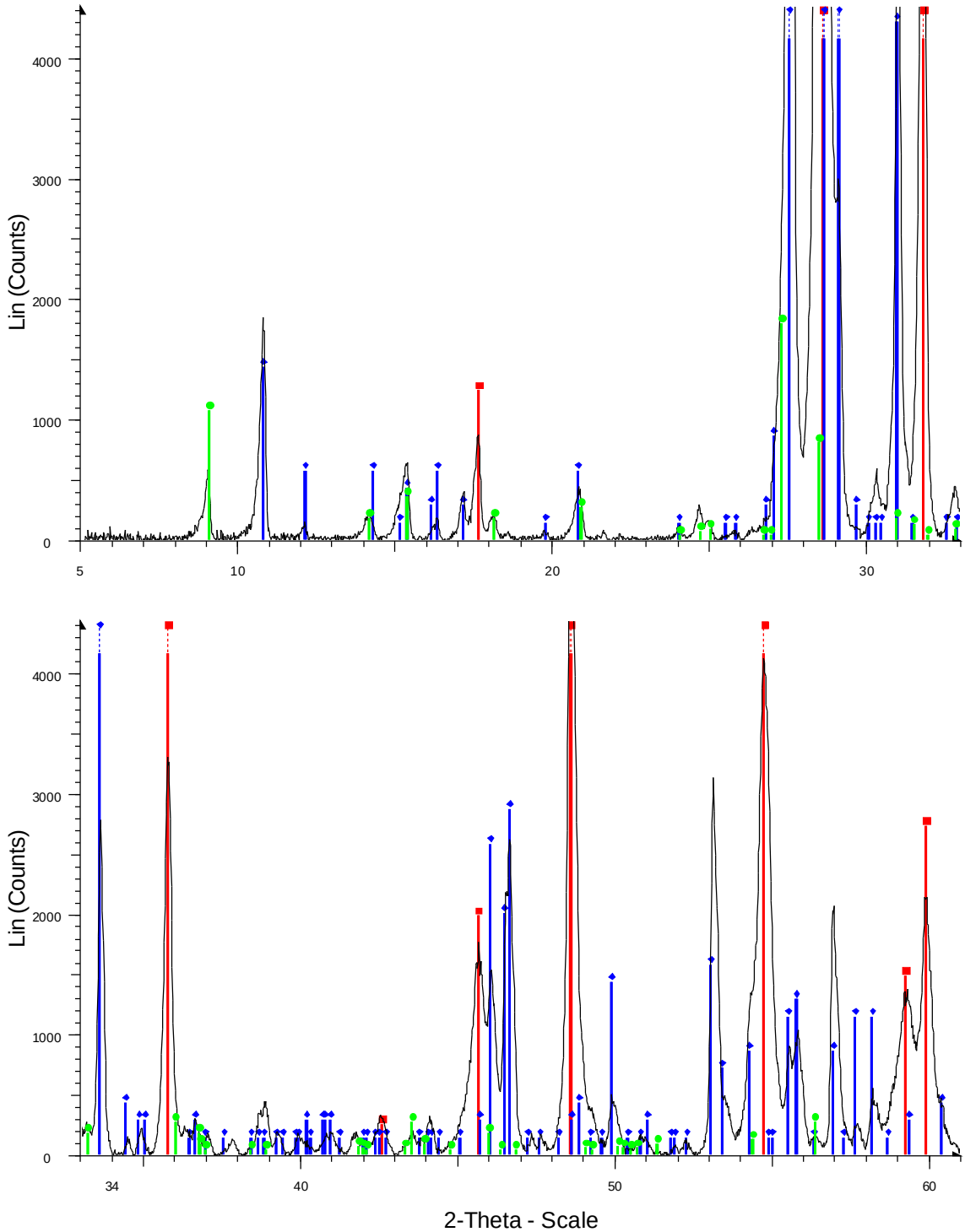
Scan: SMRR-3 (smrr-3.raw)
d multiplied by: 1.
2-theta offset: 0.000
Displacement: 0.
Criterion 3: Favor Complex Patterns
Databases: D:\PDF\PDF12-51\JCP2.CAT
Total Number: 136895
Match Chem./Subfile: 23709
Matching Intensity: 23690
Elapsed Time: 3.2

SS-NNNN	Compound Name	Mtc	nM	FOM	N°
19-1946 (N)	**Thalidomide**	**11**	**0**	**0.32**	**1**
45-1544 (*)	**6-Amino-phenalenone 6-amino-1H-phenalen-1-one**	**20**	**8**	**0.52**	**2**
48-2330 (Q)	**N-Butyl-p-nitroaniline nona(p-nitroaniline)**	**20**	**1**	**0.57**	**3**
47-2262 (I)	**Tri(benzimidazolyl)amine hydrate**	**56**	**4**	**0.59**	**4**
51-1926 (*)	Iron carbonyl sorbic acid triphenylphosphine	98	20	0.62	5
49-2430 (I)	3(2',6'-Dinitro-4'-trifluoromethyl)phenyl-thio-7,9-dimethyl- bicyclo[4.3.01,5]1	32	10	0.67	6
30-1709 (*)	1,3-Distearoyl 2-palmitoyl glycerol	43	4	0.67	7
48-2461 (*)	Cadmium diethyldithiocarbamate iodide	34	6	0.71	8
36-1887 (C)	Pentakis(aziridinyl) thiatriazadiphosphorine oxide hydrate SOaz(W)	34	2	0.71	9
23-1716 (N)	Iridium di-mu-chloro-bis(pi-cyclooctadiene-1,5)	51	8	0.73	10
30-1806 (Q)	**Methyl diphenyl-o-tolylacetate**	**22**	**7**	**0.74**	**11**
74-0777 (C)	Pentrakis(tricarbonylrutheno) methane	92	24	0.77	12
37-1658 (*)	Methyl 3-amino crotonate	39	8	0.78	13
30-1763 (I)	Iron (III) acetyl acetonate	57	12	0.79	14
47-2332 (I)	C.I. Solvent Red 1 1-[(2-methoxyphenyl)azo]-2-naphthol Sudan Red 6	33	11	0.79	15

Comments:

I have not found the selected results very convincing, but they are the best I have found despite many trials (and they are from the very first run).

DiffracPlus Eva - SMRR-4



,,,, - File: smrr-4.raw - Type: 2Th/Th locked - Start: 5.000 ° - End: 90.000 ° - Step: 0.020 ° - Step time: 1. s - Temp.: 25 °C (Room) - Time Operations: Background 0.214,1.000 | Import

05-0561 (I) - Litharge, syn - PbO - Tetragonal - Y: 100.00 %

23-0333 (*) - Lead Oxide Sulfate - Pb5O4SO4/PbSO4·4PbO - Monoclinic - Y: 57.90 %

29-0781 (*) - Lead Oxide Sulfate Hydrate - Pb4O3SO4·H2O - Triclinic - Y: 7.24 %

Search results on SMRR-4:

Search performed on all Experimental and Inorganic patterns (62,016 patterns).
Good answers from this first run are in bold characters.

Scan: ,,,, (smrr-4.raw)
d multiplied by: 1.
2-theta offset: 0.000
Displacement: 0.
Criterion 3: Favor Complex Patterns
Databases: D:\PDF\PDF12-51\JCP2.CAT
Total Number: 136895
Match Chem./Subfile: 62016
Matching Intensity: 61948
Elapsed Time: 1.3

SS-NNNN	Compound Name	Formula	Mtc	nM	FOM	N°
05-0561 (I)	**Litharge, syn**	**PbO**	**10**	**0**	**0.51**	**1**
23-0333 (*)		**Pb5O4SO4/PbSO4·4PbO**	**83**	**3**	**0.54**	**2**
50-1779 (*)		Nd2Y2O3F6	41	6	0.84	3
41-0262 (I)		Nd2.13Te1.87O6.99	59	11	0.9	4
39-0061 (*)		Bi14W2O27	20	2	0.93	5
01-0797 (D)	Litharge	PbO	7	0	1.01	6
44-0172 (*)		SrBi3VO8	36	9	1.03	7
50-0194 (I)		Bi5Pb3O10.5	29	6	1.12	8
41-0261 (I)		Pr2.22Te1.78O7.02	46	10	1.13	9
41-0755 (I)		TmF2.42	39	13	1.16	10
50-0239 (C)		PbBi12Mo5O34	96	22	1.22	11
41-0271 (I)		Nd2.67Te1.33O6.93	24	11	1.23	12
01-0796 (D)	Litharge	PbO	7	0	1.25	13
41-0754 (*)		TmF2.38	33	12	1.33	14
50-1783 (C)		Nd2Eu2O3F6	31	3	1.36	15